NOVA

Release notes previous versions

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NOVA 1.9 Release notes (Released 26/11/2012)

Introduction

Thank you for installing this update of NOVA. These notes provide an overview of the new features introduced in NOVA 1.9.

The following improvements have been added to NOVA:

- Support for 64 Bit versions of Windows
- Active profile indication in the status bar
- Hidden commands warning
- Check for updates on startup
- Linkable cutoff value in procedure editor
- Power and resistance signals added to the signal sampler
- WE(X).Charge signal added to the signal sampler
- Automatic offset DAC control
- Internal dummy cell control for the PGSTAT101 and the M101
- Optional serial number in legend
- Linkable purge time
- Procedure editor in Multi Autolab view
- iR drop correction analysis tool/command
- File extension identification in *Import GPES data* command
- Dedicated Avantes spectrometers support
- Frequencies per decade distribution in the FRA frequency scan editor
- Consolidation of the *Wait time (s)* and *Wait time (µs)* commands
- Distributed circuit element added to Fit and Simulation tool
- Clear measurement plot command

Support for 64 Bit versions of Windows

NOVA now includes support for 64 Bit versions of Windows for selected instruments. Please refer to for a list of compatible instruments (see Table 1).

Instrument type	64 Bit compatible
PGSTAT10, 20	No
PGSTAT12, 30, 302, 100	No
PGSTAT302N	Yes (Serial number ≥ AUT84440)
PGSTAT128N	Yes (Serial number ≥ AUT84460)
PGSTAT100N	Yes (Serial number ≥ AUT84500)
PGSTAT302F	Yes
PGSTAT101	Yes
Multi Autolab/M101	Yes
µAutolab II and III	No

Table 1 – Windows 64 Bit compatibility table

Active profile indication

To indicate which NOVA profiles are currently selected, indicators are now displayed on the right-hand side of the status bar. These indicators facilitate the identification of the active profile in NOVA (see Figure 1).

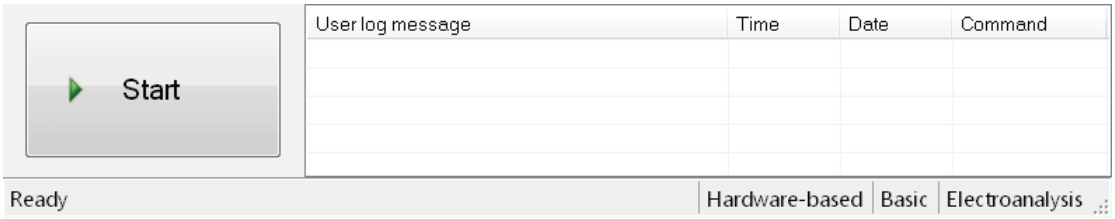


Figure 1 – Active profile indicators are now shown in the status bar

Hidden commands warning

Depending on the active profile, some commands can be hidden from view in the procedure editor: To warn the user about this, a message is now displayed in the status bar of NOVA (see Figure 2).

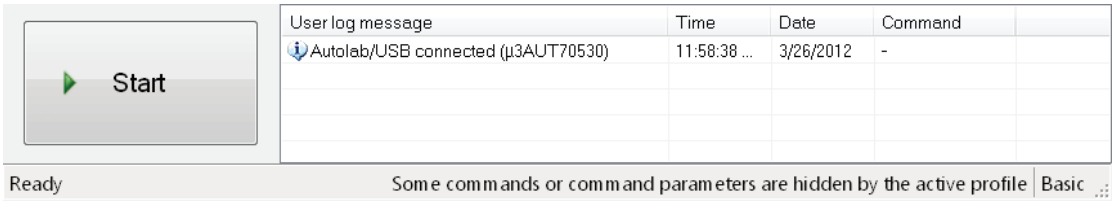


Figure 2 – A warning is shown when commands are hidden by the active profile

To reveal the hidden commands, select the Show all option from the Profile menu or adjust the active profile using the same menu.

Check for update on startup

If the computer is connected to the internet, NOVA will check if a new version is available for download from the Metrohm Autolab website on startup. If a new version is available, an indication will be displayed in the connection manager in the lower right corner of the screen (see Figure 3).

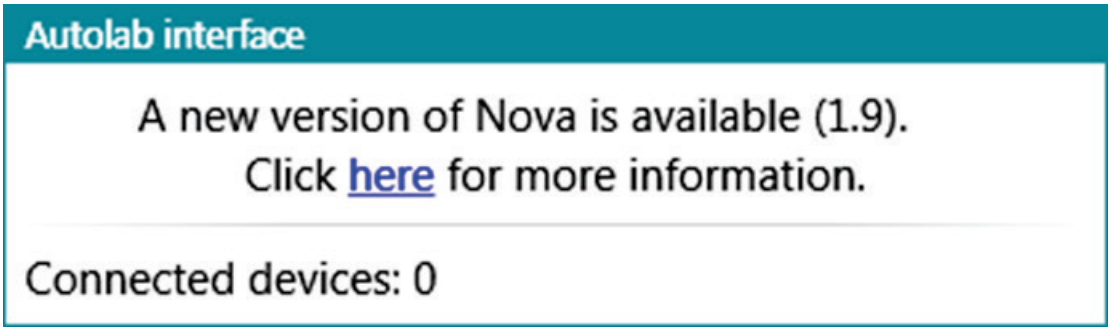


Figure 3 – A message is show when a new version if available for download

Linkable cutoff value in procedure editor

The value parameter used in the Cutoff option, can now be linked in the procedure editor if a unique identifying name is given to it. The Edit Options window now provides an additional field on the Cutoff tab, allowing the user to specify the name of the parameter to use in the procedure editor to identify the cutoff limit (see Figure 37).

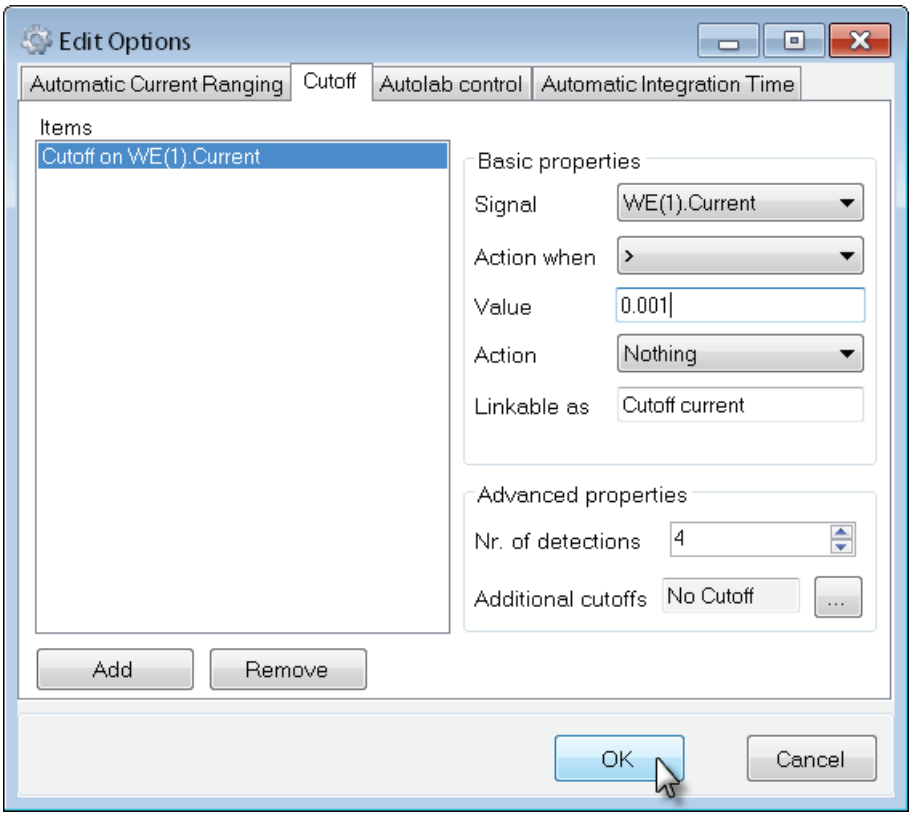


Figure 4 – The value of the cutoff is now linkable if a name is provided on the Cutoff tab

If a name is provided in the *Linkable as* field in the basic properties, this parameter will be shown in the procedure editor (see Figure 5). Other command parameters can then be linked to this parameter, which allows the cutoff value to be modified or specified by other commands, while the measurement is running (using an input box or a calculate signal, for example).

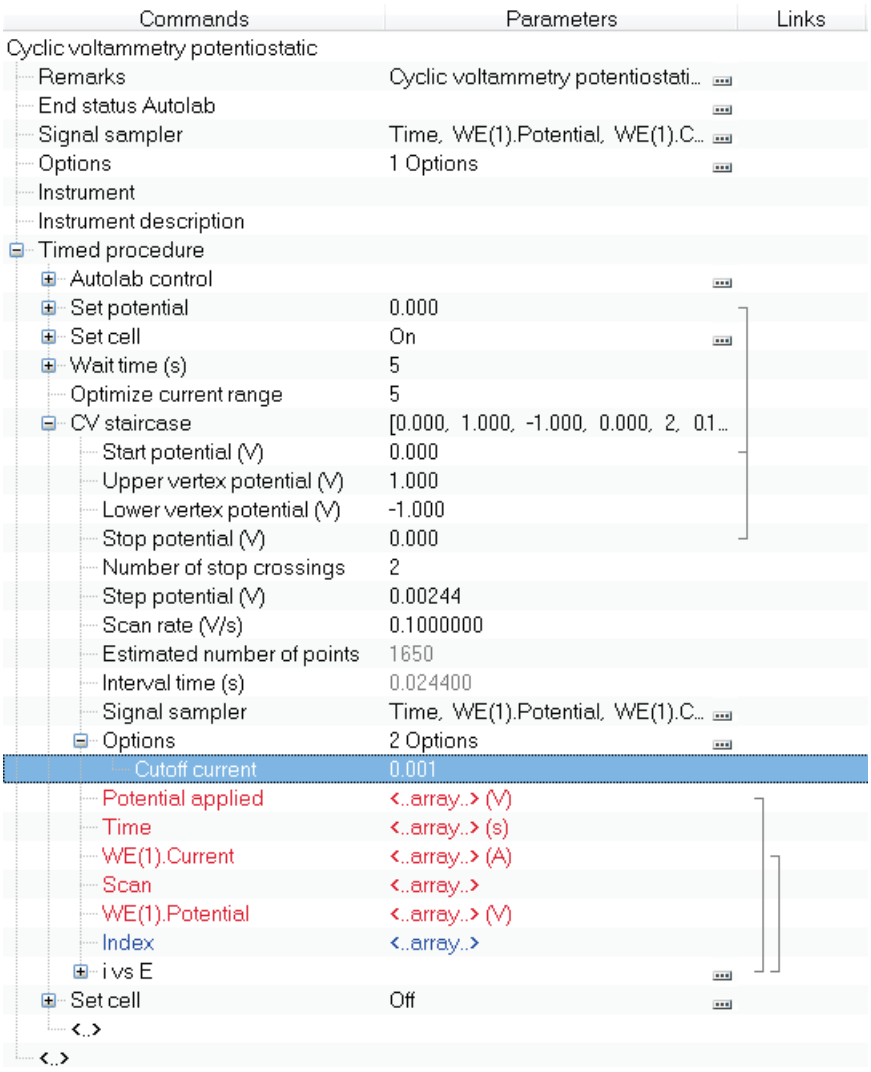


Figure 5 – The cutoff limit is displayed in the procedure editor if a name is provided

Power and Resistance signals

The WE(1).Power signal (in Watt) and the WE(1).Resistance signal (in Ohm) have been added to the signal sampler. These signal are derived from the WE(1).Potential and the WE(1).Current signals and can only be recorded if both signals are sampled (see Figure 38).

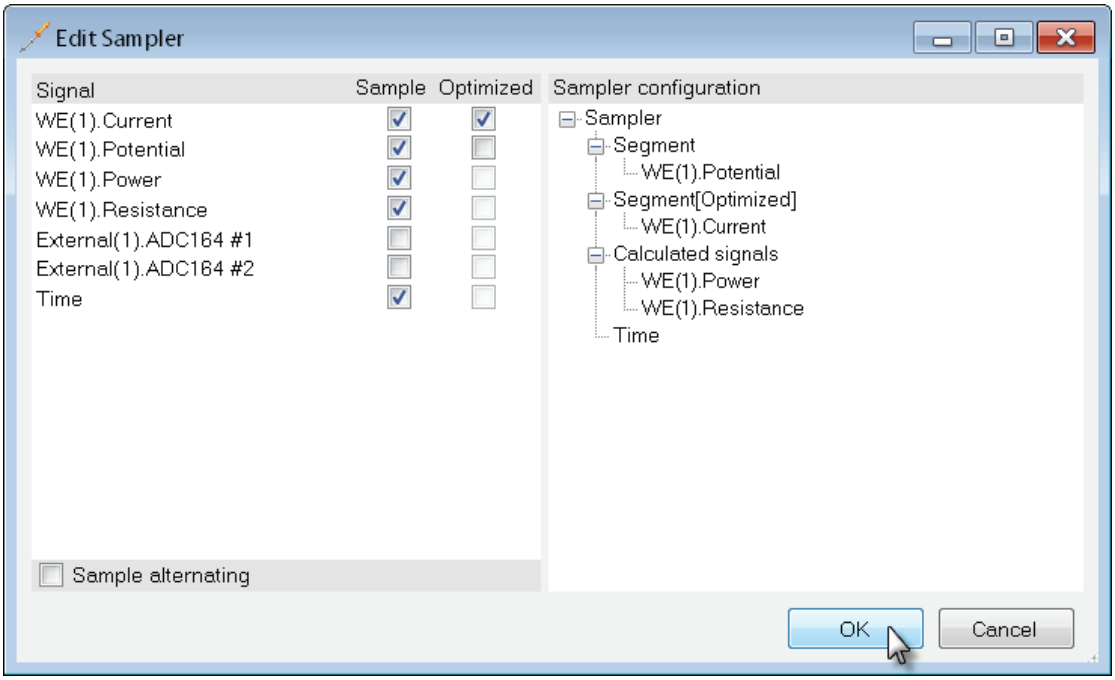


Figure 6 – WE(1).Power and WE(1).Resistance signals are now available in the sampler

These new signals are calculated signals and therefore cannot be sampled in *optimized* mode. The calculation is performed in real time, which allows these new signals to be involved in the cutoff option as well (see Figure 7).

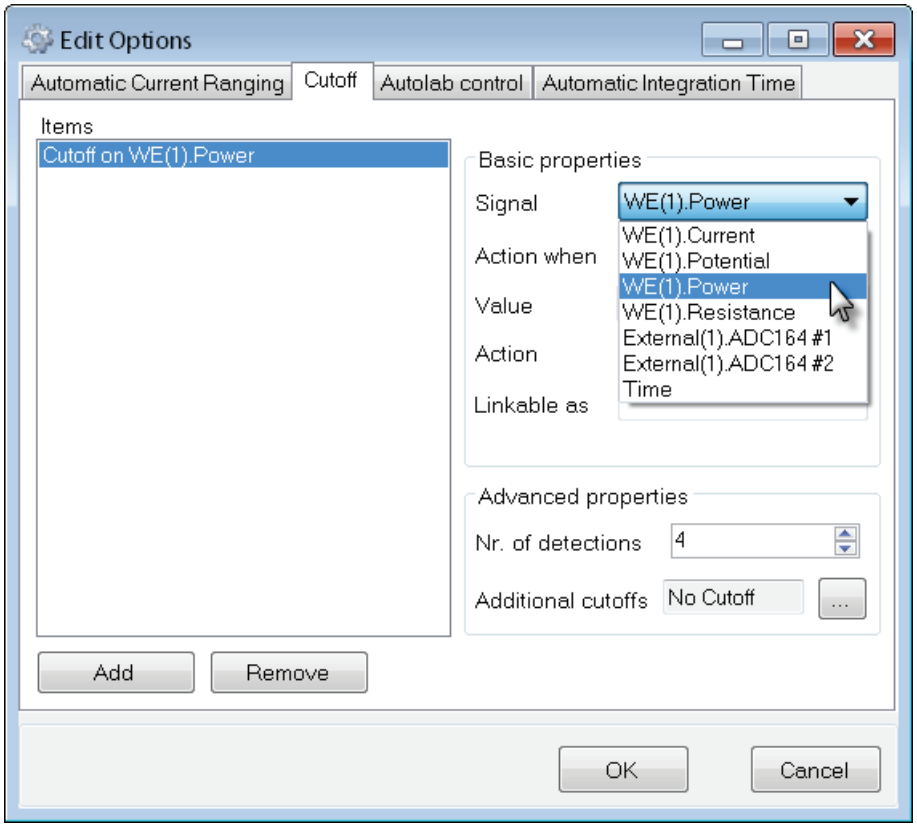


Figure 7 – The new signals are also available in the cutoff option

WE(X).Charge signal

The WE(X).Charge signal (in Coulomb) has been added to the signal sampler. This signal is available for each working electrode for which the current signal is measured (see Figure 8).

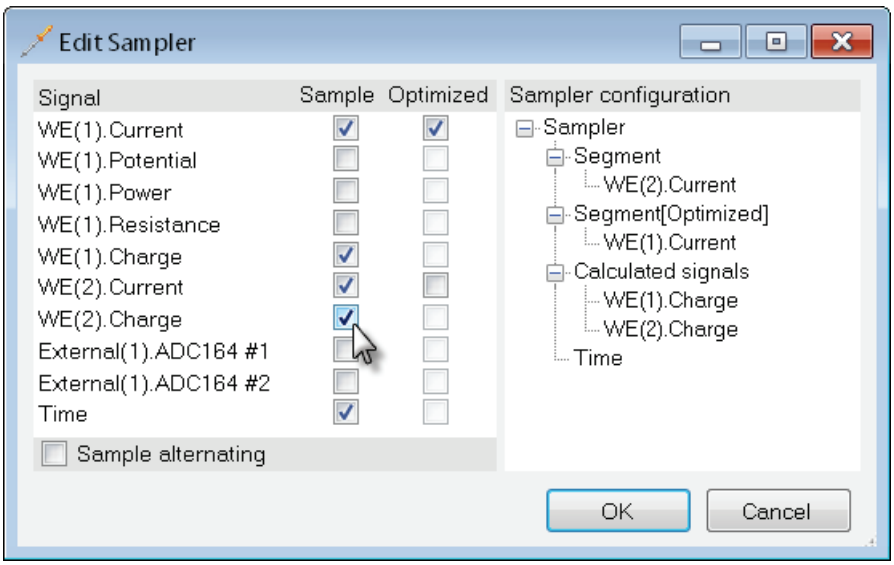


Figure 8 – WE(X).Charge signals are now available in the sampler

The WE(X).Charge signal is a calculated signal and therefore cannot be sampled in *optimized* mode. The calculation is performed in real time, which allows these new signals to be involved in the cutoff option as well (see Figure 9).

Warning

The charge is calculated mathematically using the so-called trapezoidal method. The accuracy of this method depends on the interval time and on the current derivative. In most cases, the calculated charge will only be a first approximation of the real charge, which can be measured properly using the optional FI20 module or the on-board integration.

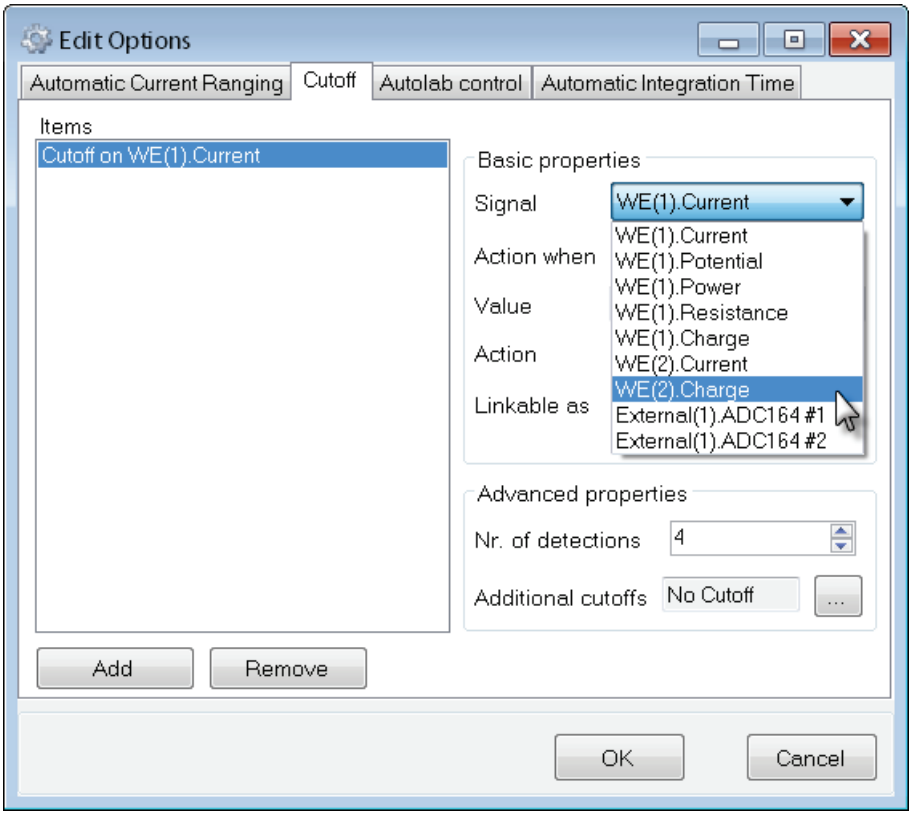


Figure 9 – The calculated charge is available in the cutoff option

Automatic offset DAC control

The offset DAC, described in Chapter 4 of the NOVA Getting started manual, is now automatically set by the software, whenever required. This allows the potential or the current to be set automatically to any value within the applicable range.

Note

The offset DAC should not be modified when the cell is on during a measurement. A warning is provided during validation if the procedure requires the offset DAC to be reset during the experiment (see Figure 7).

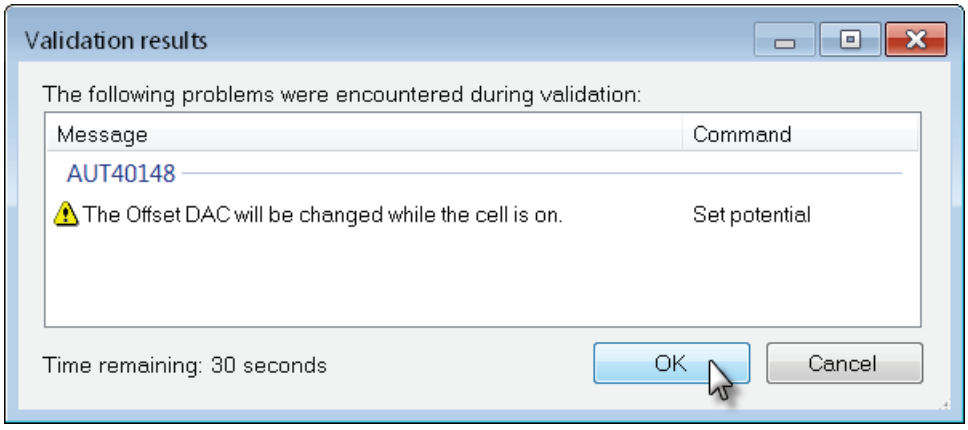


Figure 10 – A warning is provided when the offset DAC is reset while the cell is switched on

Internal dummy cell control for PGSTAT101 and M101

The PGSTAT101 and M101 are both fitted with an internal dummy cell. This internal dummy cell can now be controlled through the *Autolab control* command, as shown in Figure 64.

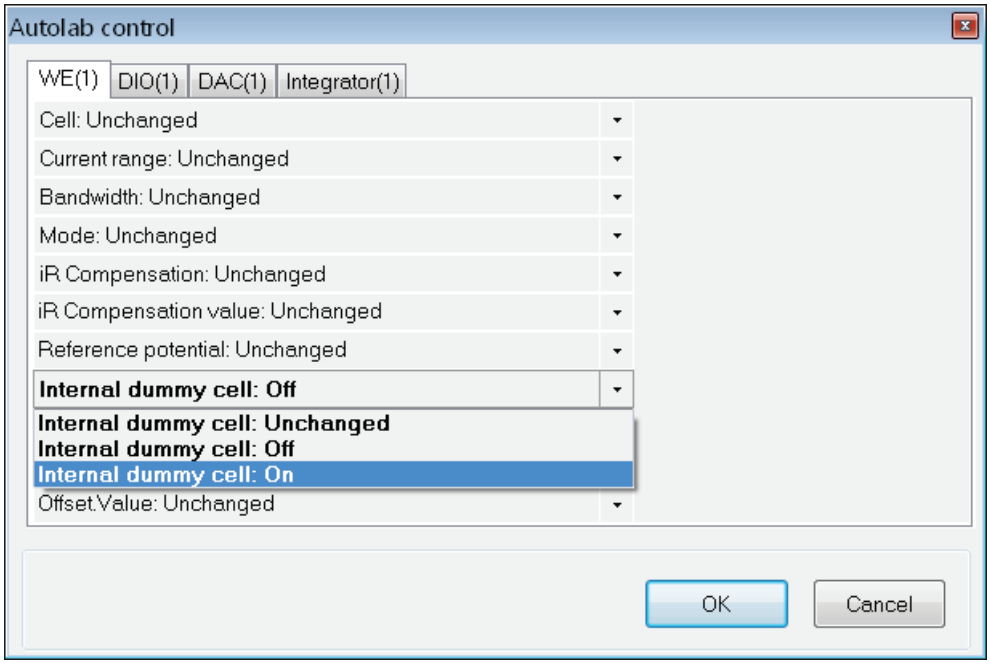


Figure 11 – The internal dummy cell for the PGSTAT101 and the M101 can now be controlled using the *Autolab control* command

Using the internal dummy cell toggle, it is possible to set the internal dummy cell on or off.

Note

The internal dummy cell must be switched off when measurements are performed on a real cell. The procedure validation will always provide a warning when a measurement is started with the internal dummy cell on (see Figure 12).

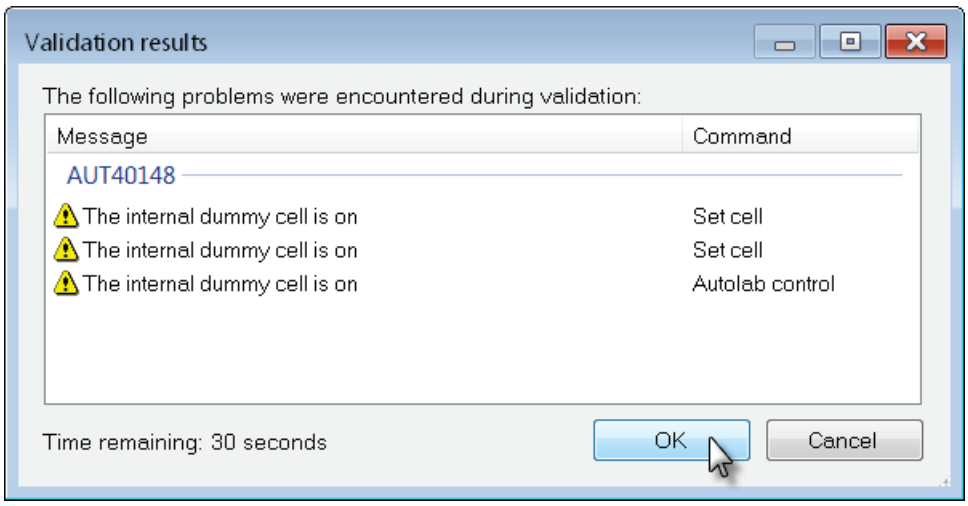


Figure 12 – A warning is provided during validation when the internal dummy cell is on

Optional serial number in legend

By default, the Autolab serial number is displayed in the legend of any plot to facilitate the identification of the instrument in an overlay plot. It is now possible to deactivate this option through the NOVA options (see Figure 13).

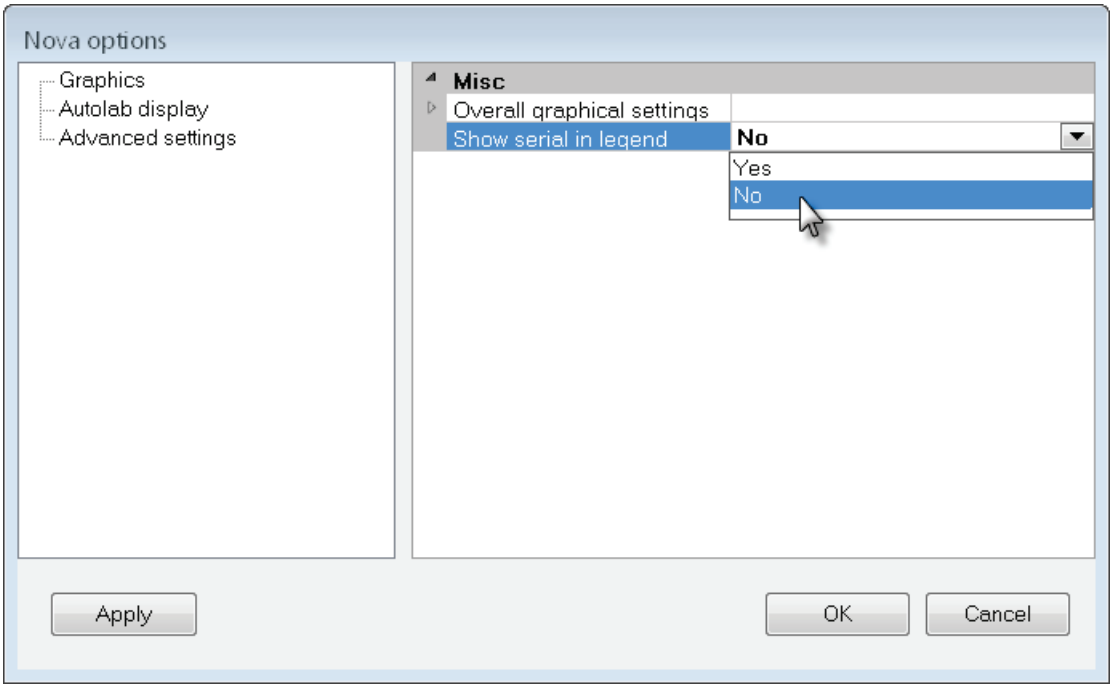


Figure 13 – The NOVA options allow the serial number to be activated or deactivated in the legend

Linkable purge time

The Duration parameter of the *Purge time* command is now linkable to other command parameters (see Figure 47).

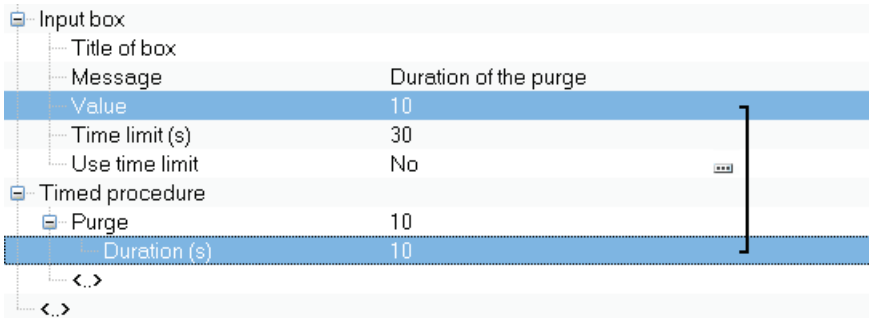


Figure 14 – The duration parameter of the *Purge time* command is now linkable

Procedure editor in the Multi Autolab view

To facilitate editing of multiple procedures in the Multi Autolab view, a simplified procedure editor is available in this view to edit existing procedures. To open this editor, click the Edit button located next to the specified path (see Figure 66).

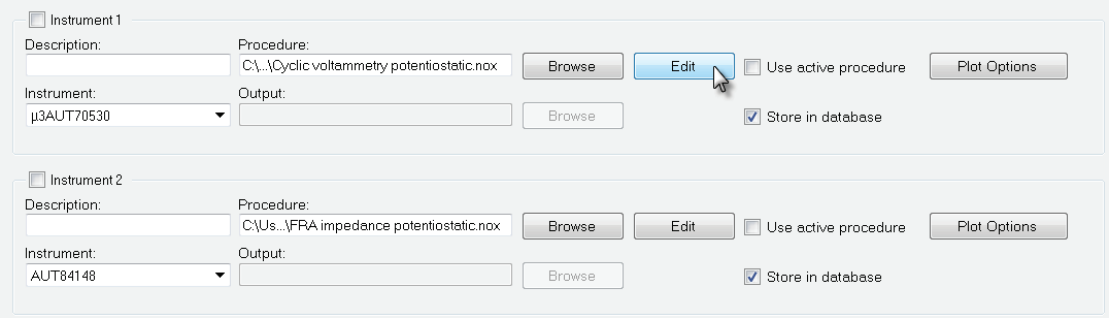


Figure 15 – Clicking the Edit button in the Multi Autolab view opens a simplified procedure editor

Clicking the Edit button opens a popup window displaying a reduced form of the setup view. Through this window, the procedure can be modified. Commands and links in the procedure can be edited and the changes can be saved to file (see Figure 16).

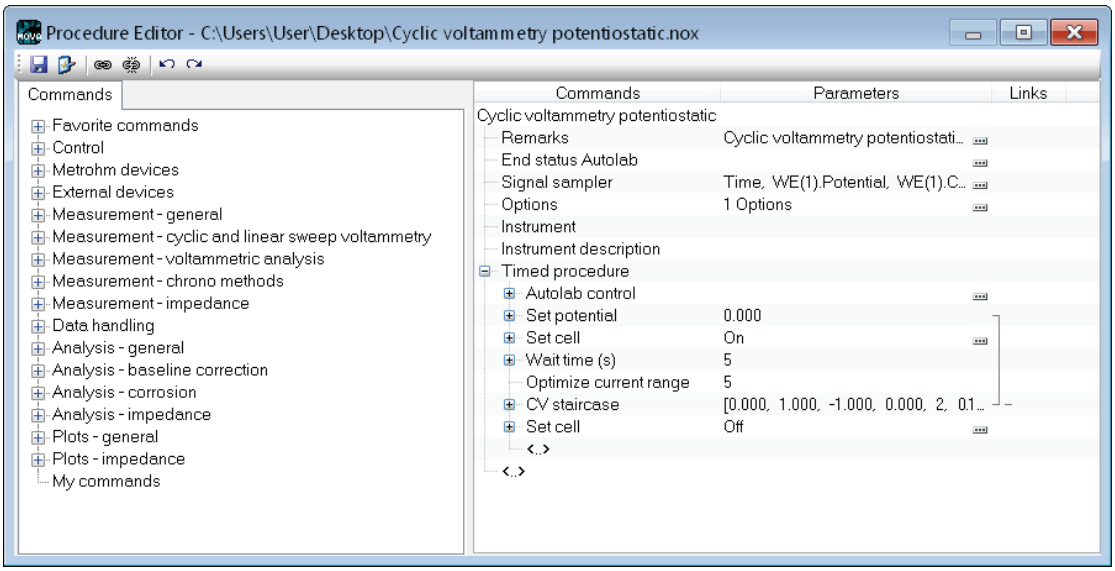


Figure 16 – A simplified view of the setup view is shown when the Edit button is clicked

iR drop correction tool

The *iR drop correction* command and analysis tool have been added. This tool can be used to automatically correct the data, after the measurement is finished, for iR drop. This tool requires the user to manually set the value of the uncompensated resistance to use in the calculation.

The tool calculates an adjusted value of the applied potential, given by:

$$E_{Corrected} = E_{Applied} - iR_u$$

Where R_u is the resistance value specified by the user. The command can be found in the analysis – general group of commands. The analysis tool can be added to a measured data set directly (see Figure 17).

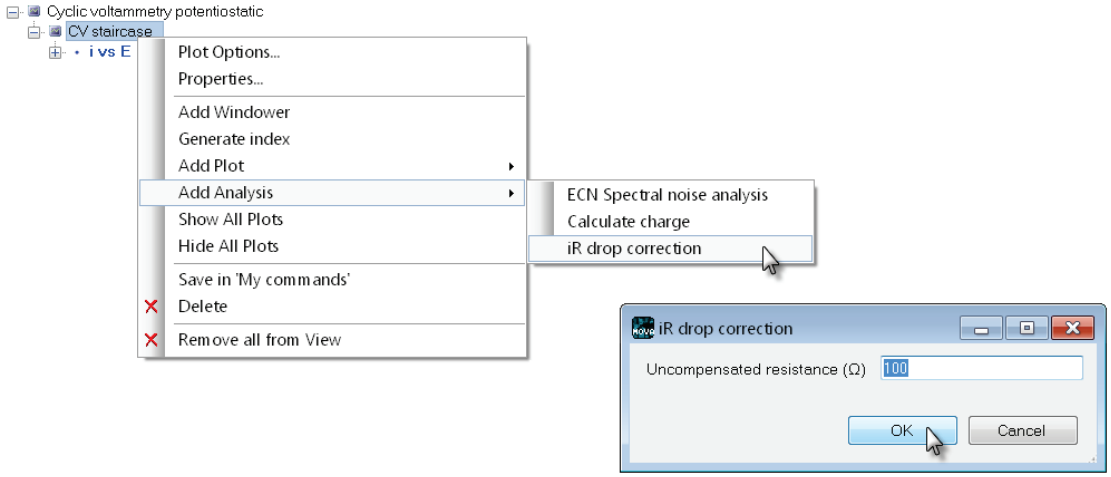


Figure 17 – The iR drop correction analysis tool allows to correct the data for iR drop after the measurement

The *Corrected potential* signal is added to the original data after the calculation. After the calculation, the corrected data can be plotted (see Figure 18).

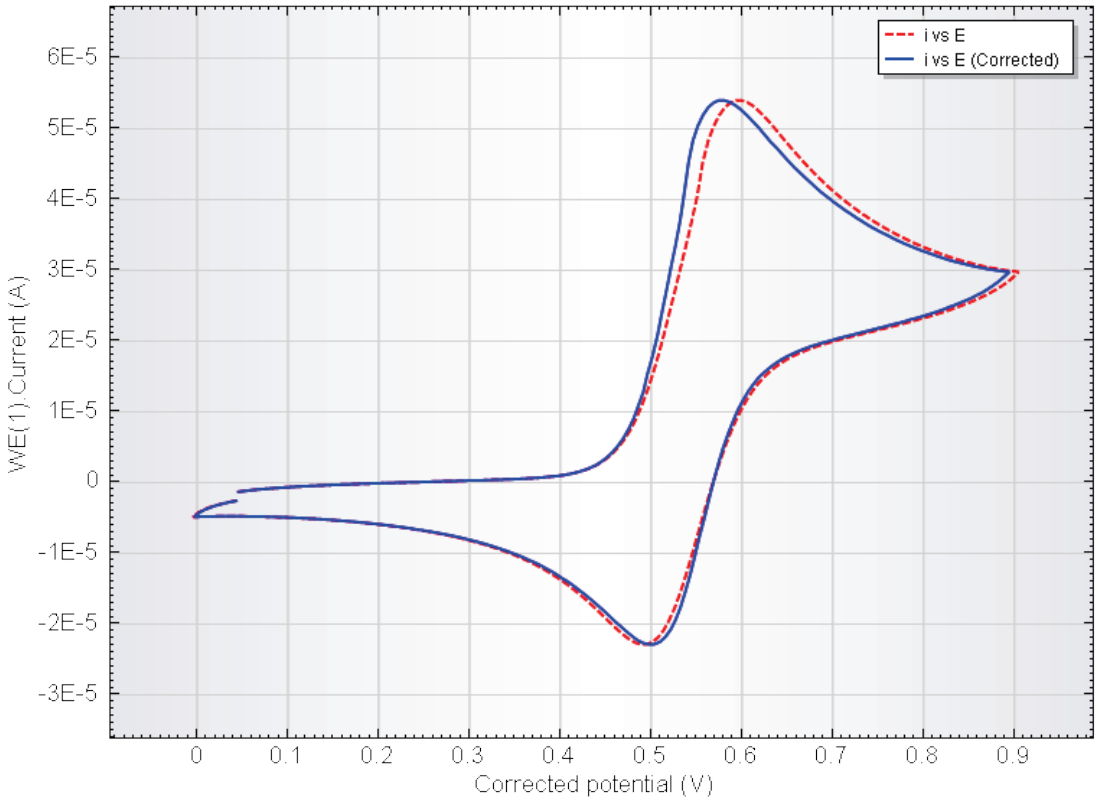


Figure 18 – The *iR drop correction* command can be used to correct the measured data for ohmic drop

File extension identification in Import GPES data command

The *Import GPES data* command has been modified in order to recognize the extension of the file and assign the suitable signal names to the imported data[1]. Depending on the file extension of the specified file, NOVA will import the data as detailed in Table 2.

Extension	Type of data	Signals	Plots
.ocw	Cyclic voltammetry, Linear sweep voltammetry	i, E	i vs E
.oxw	Chrono methods	i, t	i vs t
.oew	Voltammetric analysis	i, E	i vs E
.opw	Potential stripping analysis	E, dt/dE	dt/dE vs E
.onw	Electrochemical noise	E, i, t	E vs t
.odw	Multimode electrochemical detection	i, t	i vs t

Table 2 – Overview of the identifiable GPES file extensions

Avantes spectrometers support

USB 2.0 controlled Avantes AvaSpec spectrophotometers are now directly supported in NOVA. The Avantes instruments can be controlled by NOVA in combination with the Autolab. The commands related to the control of the Avantes instruments have been added to the External devices group of commands (see Figure 19).

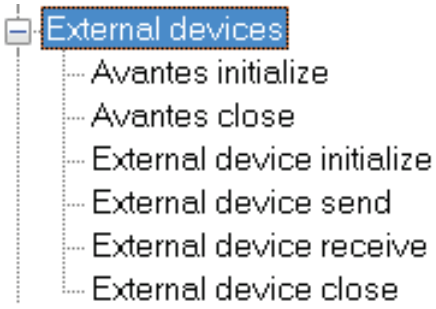


Figure 19 – Dedicated commands to control Avantes spectrometers are available in the External devices group of commands

[1] Please refer to the GPES User Manual for more information on the file format of the GPES files.

Two commands are available:

- **Avantes initialize:** initializes the control of a specified Avantes spectrophotometer connected to the computer. This command can be used to specify the measurement range, the integration time and other data acquisition parameters for the spectrophotometer.
- **Avantes close:** terminates the control of the initialized Avantes spectrophotometer and recovers the measured data from the spectrometer. This data is then associated with electrochemical data from the Autolab, if applicable.

Frequencies per decade in the FRA frequency scan editor

It is now possible to specify the frequencies per decade to use in a FRA frequency scan rather than the absolute number of frequencies in the scan. When the number of frequencies per decade is specified, a logarithmic distribution is used between the first and last specified frequencies (see Figure 20).

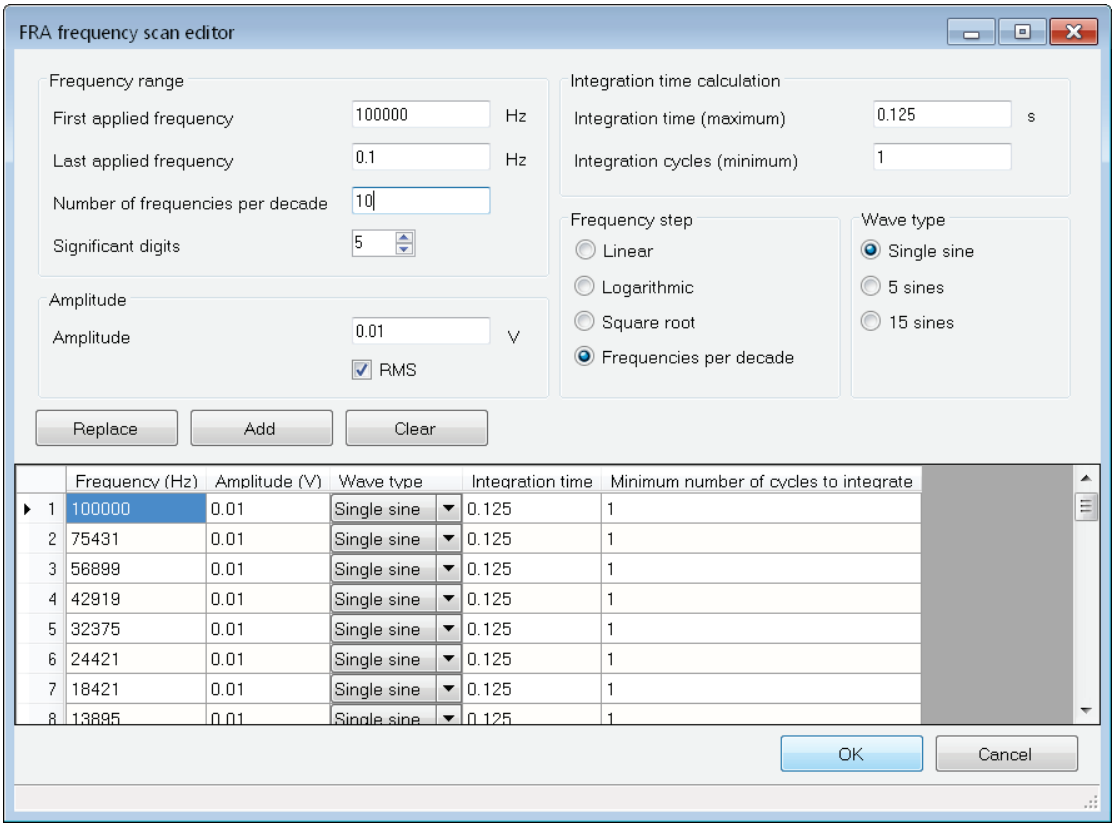


Figure 20 – It is now possible to define the frequency scan using a Frequency per decade distribution

Using this distribution, the actual number of frequencies is defined by the First and Last applied frequencies in the scan.

Merge files option

It is now possible to merge files in order to generate a new file which contains the data from the source files. This option can be used when data included in one file needs to be used in a calculation involving data from another file. The source files are not deleted and a new file is created instead. A name for the new file must be specified upon merging (see Figure 21).

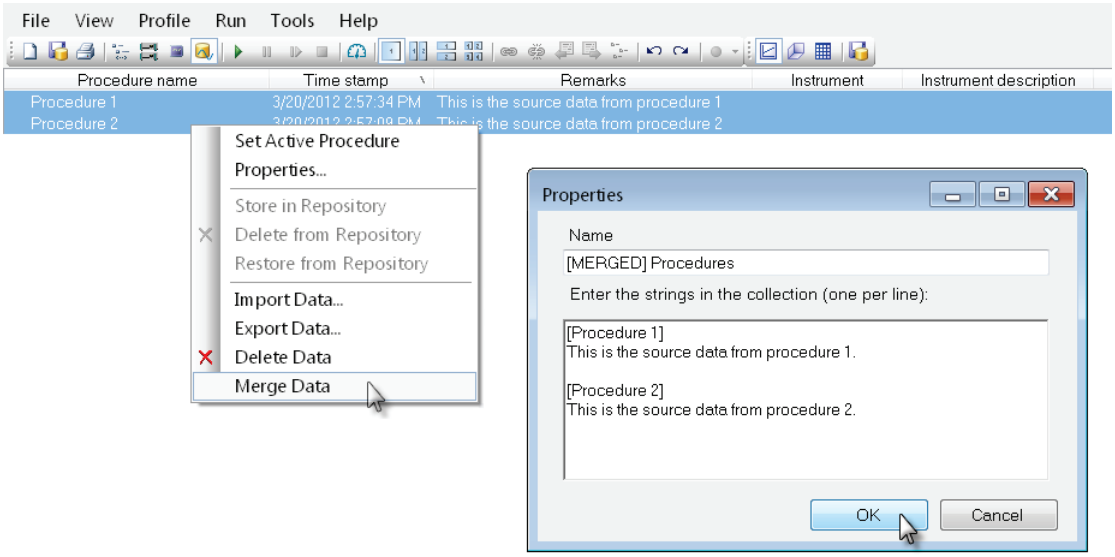


Figure 21 – Merging data files in the NOVA database

A new file is created and added to the database. This file contains the data from the merged source files (see Figure 22).

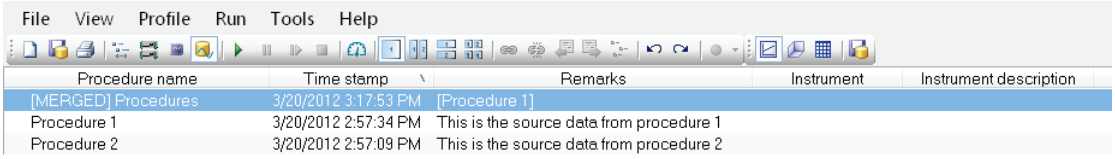


Figure 22 – A new merged file is added to the database

Wait time and Wait time (µs) command consolidation

The Wait time (s) and Wait time (µs) commands have been consolidated to avoid confusion. Both commands are now replaced by a single Wait time (s) command which accepts decimal values. The accuracy of the wait time is ~ 1 ms.

New circuit element for Fit and Simulation

The library of circuit elements has been expanded by adding the B2 circuit element.

The B2 circuit element available in the Fit and Simulation analysis tool is a transmission line element derived from the classical model for a porous or mixed-phase electrode of thickness L (see Figure 23).

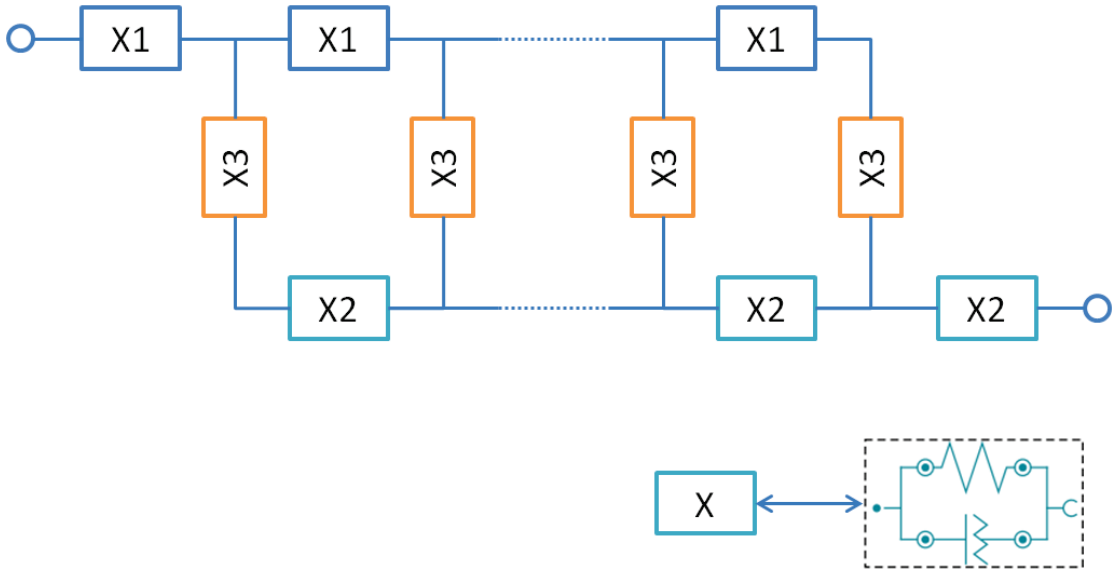


Figure 23 - Overview of the B2 circuit element

This transmission line has been integrated in NOVA. In the literature, this denomination is also extended in the world of DSC and in general systems that analyze the combination of charge transport, accumulation and recombination.

More information on the B2 circuit element can be found in the Appendix of the Impedance measurements tutorial, available in the Help menu in NOVA.

Clear measurement plot command

A *Clear measurement plot* command has been added to the Control group of commands (see Figure 24).

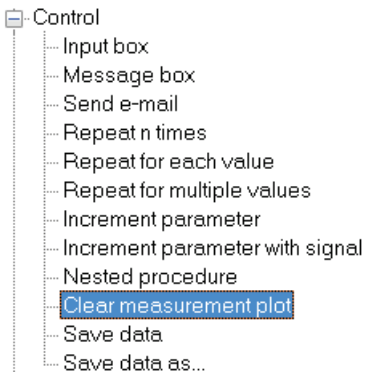


Figure 24 – The *Clear measurement plot* command has been added to the Control group of commands

This command can be added anywhere in the procedure to clear the contents of one of the four available plots, or all plots at once.

NOVA 1.8 Release notes (Released 01/12/2011)

Introduction

These notes provide an overview of the new features introduced in NOVA 1.8 compared to the previous release.

The following items have been added to this release of NOVA:

- Support for the instruments and modules:

  - FRA32M – New impedance analyzer module

- Improvements and additions:

  - Automatic update tool for USB interfaces
  - Automatic Hardware setup
  - Simplified interface with Profile menu
  - Hide/Show option
  - Sorting function for the Commands browser
  - Import/Export Profiles
  - Context sensitive popup menu
  - Add comments to *My Commands*
  - Favorite commands group
  - Basic Undo/Redo functionality
  - Modification to the *Calculate signal* command
  - Noise meters added to Autolab display
  - Real time modification of the command parameters
  - Add plots in real time
  - Modification of the plot options in real time
  - Create Windower from X axis
  - New plot options
  - Linkable interval time in *Record signals (> 1 ms)* command
  - Pseudo capacitance calculation for (RQ) circuit

Automatic update tool for USB interfaces

Autolab PGSTAT302N and PGSTAT100N with serial numbers > AUT84440 and PGSTAT128N with serial numbers > AUT84460 need a firmware update to avoid a potential USB communication problem. This update is only required for the above mentioned instruments when used in combination with the NOVA only drivers.

An automatic update tool is included in the Diagnostics application.

Note: when NOVA is used with the instruments mentioned above in combination with the NOVA only driver, the initialization of the instrument will be stopped until the firmware is updated (see Figure 25).

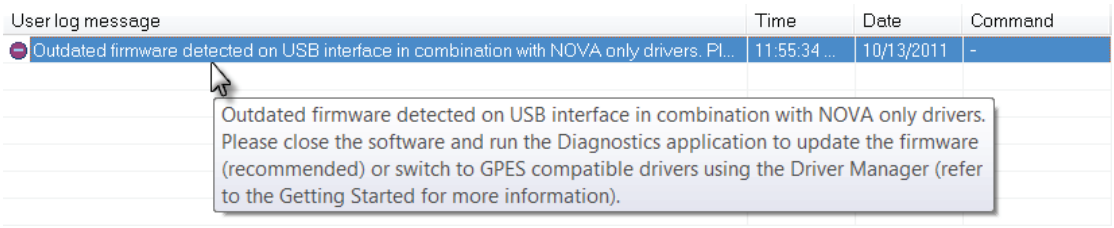

User log message
Time
Date
Command
Outdated firmware detected on USB interface in combination with NOVA only drivers. Pl...
11:55:34 ...
10/13/2011
-
Outdated firmware detected on USB interface in combination with NOVA only drivers. Please close the software and run the Diagnostics application to update the firmware (recommended) or switch to GPES compatible drivers using the Driver Manager (refer to the Getting Started for more information).

Figure 25 – The initialization of the instrument is blocked when the outdated firmware is detected on an instrument controlled through the NOVA only driver

During Diagnostics, an update message will be displayed if the outdated firmware is detected. Clicking the Yes button when prompted will silently update the firmware (see Figure 26).

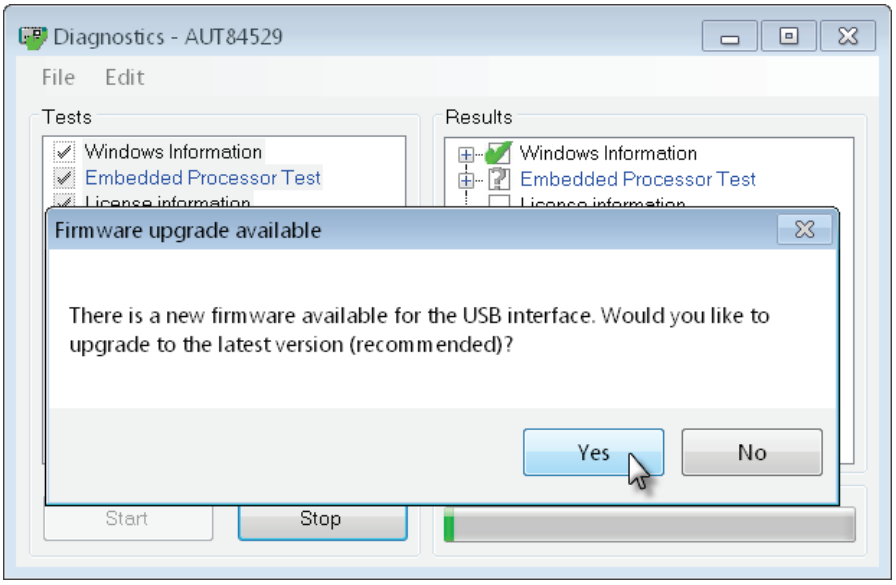


Figure 26 – An upgrade message is displayed when the outdated firmware is detected

The firmware update is permanent and needs to be carried out only once. The update will take about five seconds.

FRA32M

The FRA32M is the new impedance analyzer module for the modular Autolab PGSTAT instruments and the Multi Autolab instruments. It replaces the FRA2 module and it is compatible with all the commands and procedures used in combination with the FRA2 module.

The FRA32M is fitted with a frequency generator that reaches 32 MHz. However, when the FRA32M is used in combination with the Autolab PGSTAT, the maximum frequency that can be applied in a measurement is 1 MHz[2]. For measurements involving external devices, the frequency can be increased.

[2] The maximum frequency that can be used in combination with the FRA32M depends on the highest achievable bandwidth of the Autolab PGSTAT. Please refer to the Getting started manual for more information.

Please refer to the Impedance spectroscopy tutorial, available from the Help menu, for more information.

Automatic Hardware setup

Whenever an Autolab is connected to the computer for the first time, Nova will try to configure the instrument automatically by reading out the on-board EEPROM information. This allows the software to pre-configure the hardware setup without user-intervention.

For old instruments and old modules[3], this automatic configuration can sometimes not be done accurately. For this reason it is always recommended to verify that the configuration is accurate after initialization of the instruments.

Simplified interface with Profile menu

A profiling scheme has been added to Nova. Using this tool, it is possible to hide some commands in order to simplify the user interface. The profiles can be adjusted using the dedicated Profile menu (see Figure 27).

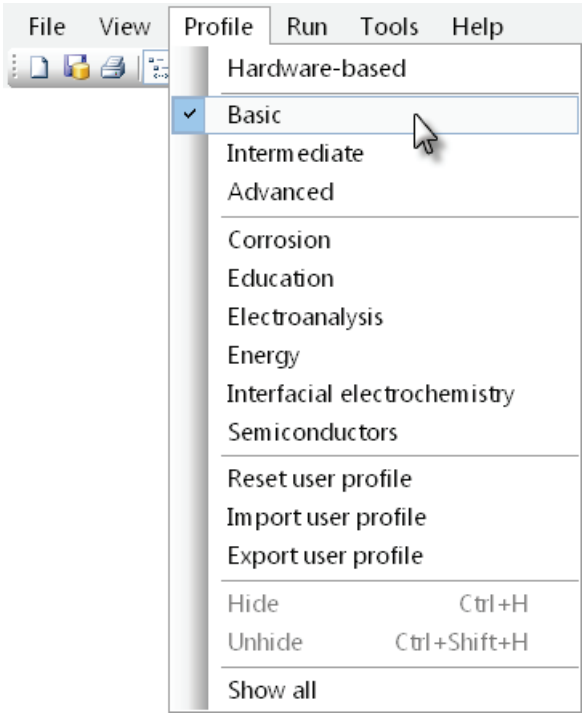


Figure 27 – The profile menu can be used to set the user profile

The profiles are grouped in three sections:

- Level based (mandatory, set to Intermediate by default)
- Hardware based (optional)
- Application based (optional)

[3] Please refer to the Getting started manual for more information.

Level based

All the commands and the procedures in Nova have been tagged with three levels: basic, intermediate and advanced. When the basic profile is active, only a few simple commands are shown, when the advance profile is active, all the commands are shown (see Figure 28).

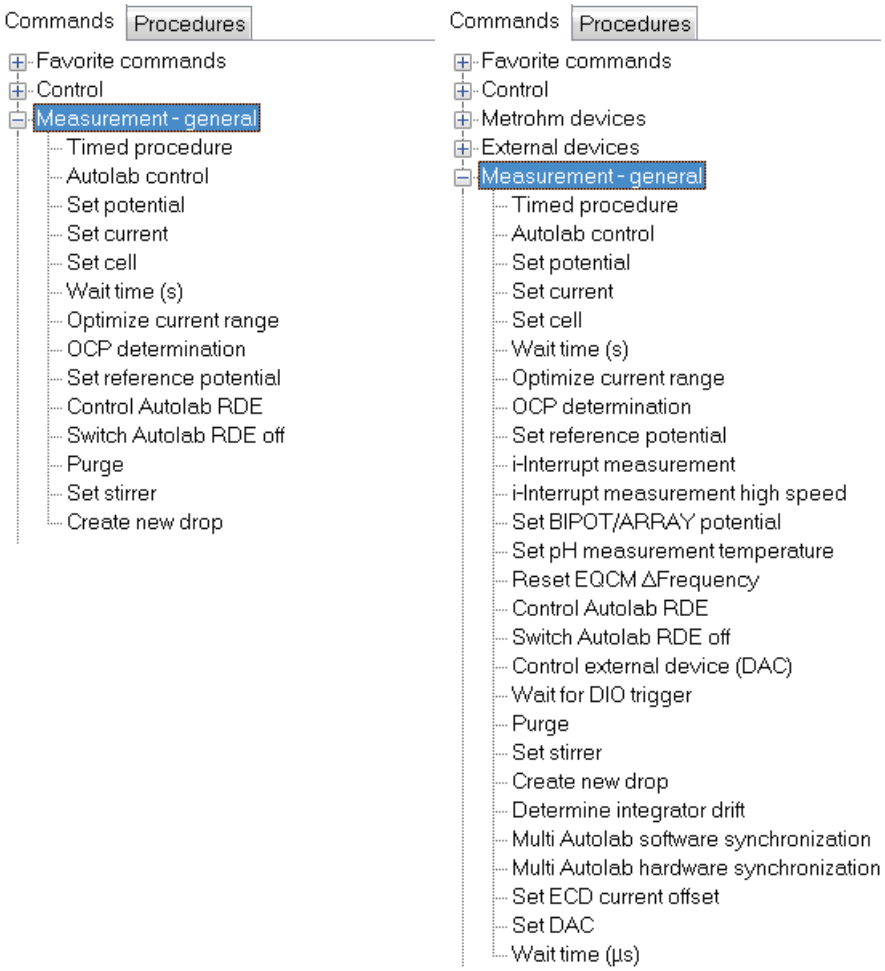


Figure 28 – Difference between the basic (left) and the advanced (right) profile

Note: the **intermediate** profile is the default level based profile selected upon installation of Nova.

Important: the selected level based profile is always on.

Hardware based

All the commands and the procedures in Nova have been tagged with a hardware requirement marker. When the hardware-based profile is active, only the procedures and commands that can be executed with the connected instrument are shown. In Figure 29, the Autolab procedures are shown without and with the hardware-based profile active, for a µAutolabIII. Since the µAutolabIII is not fitted with the required hardware, several procedures are hidden.

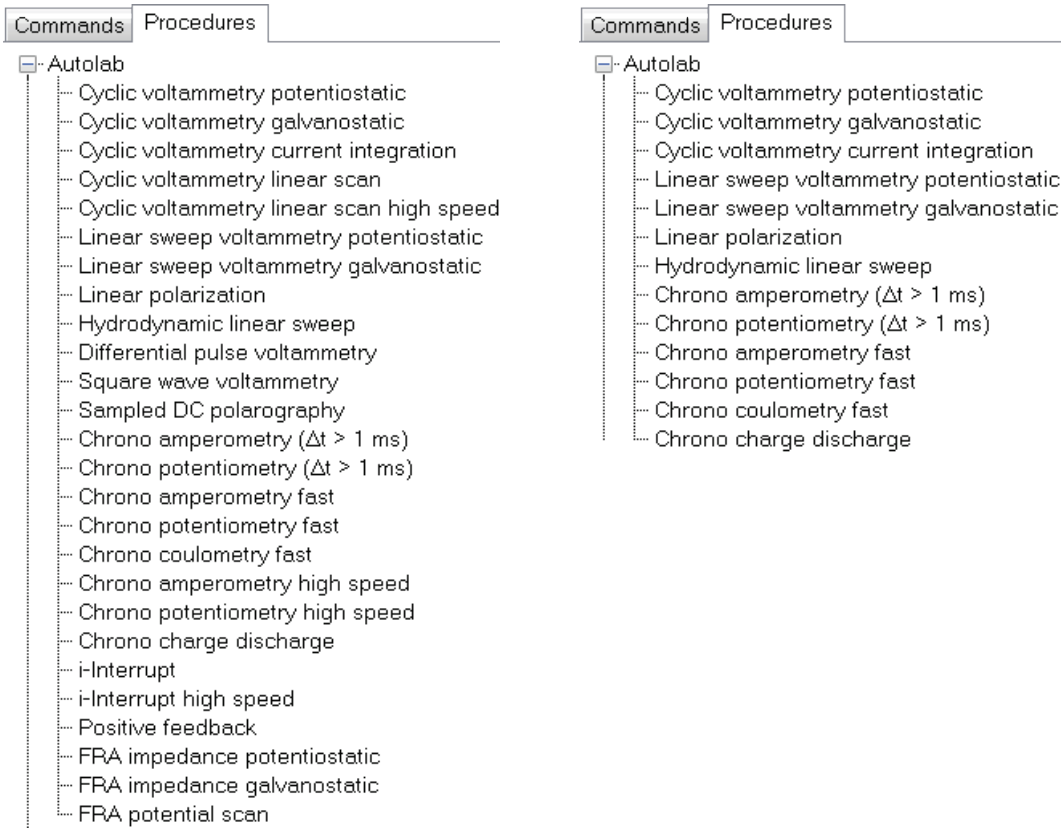


Figure 29 – Overview of the Autolab procedures with a µAutolabIII (left, hardware-based profile not active and right, hardware-based profile active)

Application based

All the commands and the procedures in Nova have been tagged with an application marker: corrosion, energy, electroanalysis, etc... When a given application profile is active, only the commands and procedures relevant for this application are shown (see Figure 30).

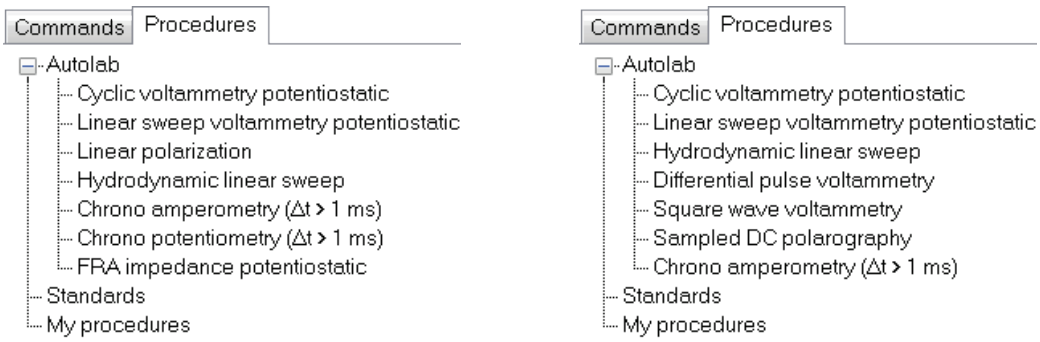


Figure 30 – Difference between the corrosion (left) and the electroanalytical (right) profile

Note: it is possible to combine all the profile schemes at the same time. For example, it is possible to set the profile to show hardware-based and intermediate commands and procedures for the energy application (see Figure 31).

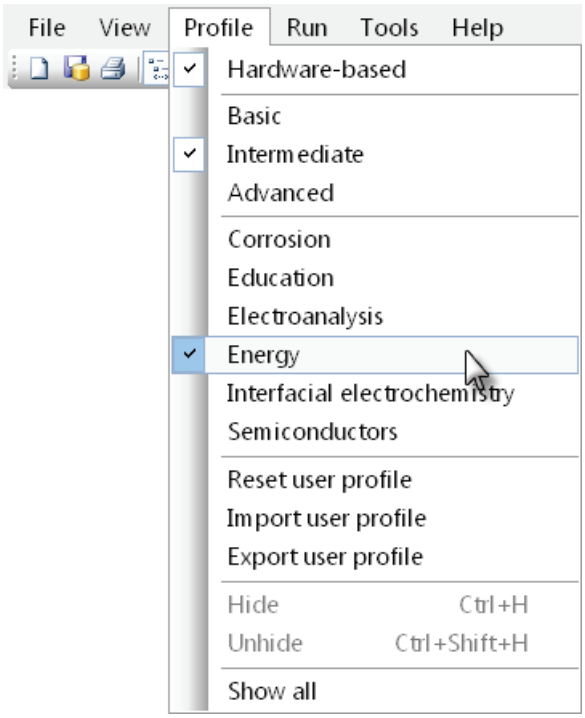


Figure 31 – It is possible to combine several profiles at the same time (intermediate, hardware-based and energy related)

Hide/Show option

To further customize the appearance of the user interface, the option to hide and show procedures, commands, and command parameters has been added. To hide an item in Nova, simply right-click the item and select the hide option from the menu. In Figure 32, this option is used to hide the *Chrono coulometry fast* procedure from the procedures browser.

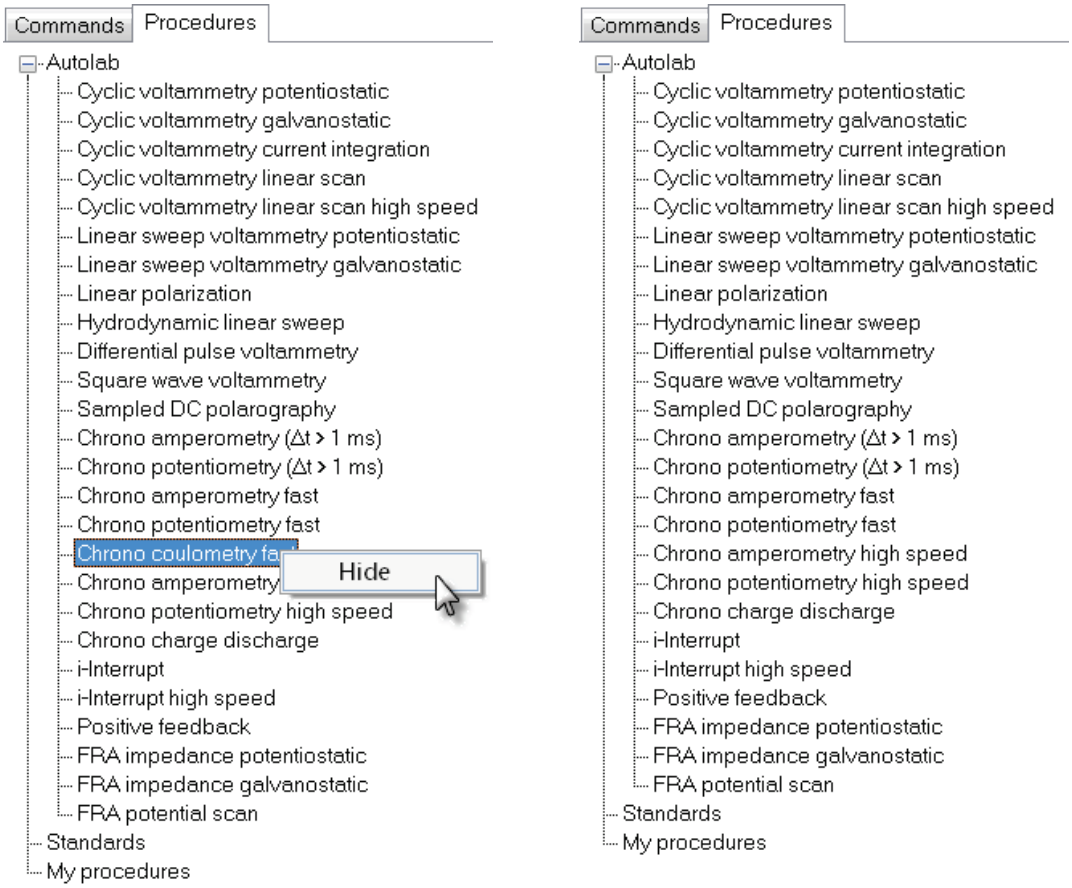


Figure 32 – Hiding a procedure from the procedure browser

Once an item has been hidden from view, it will not be shown until it is unhidden. To unhide hidden commands, procedures or command parameters, select the Show all option from the Profiles menu (see Figure 33).

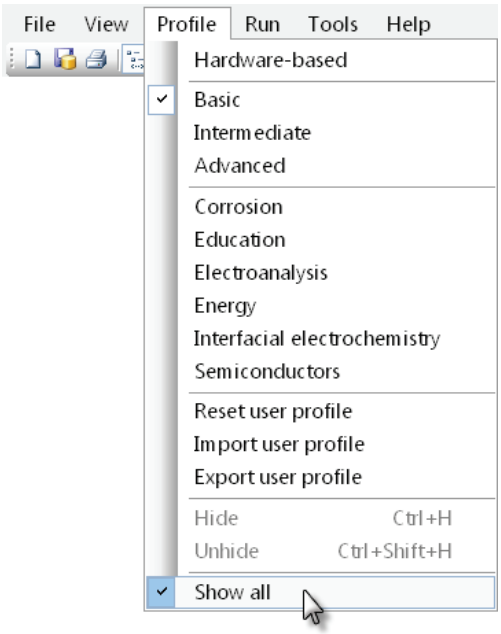


Figure 33 – Select the Show all option from the Profile menu to display all hidden items

Hidden items are shown in green (see Figure 34).

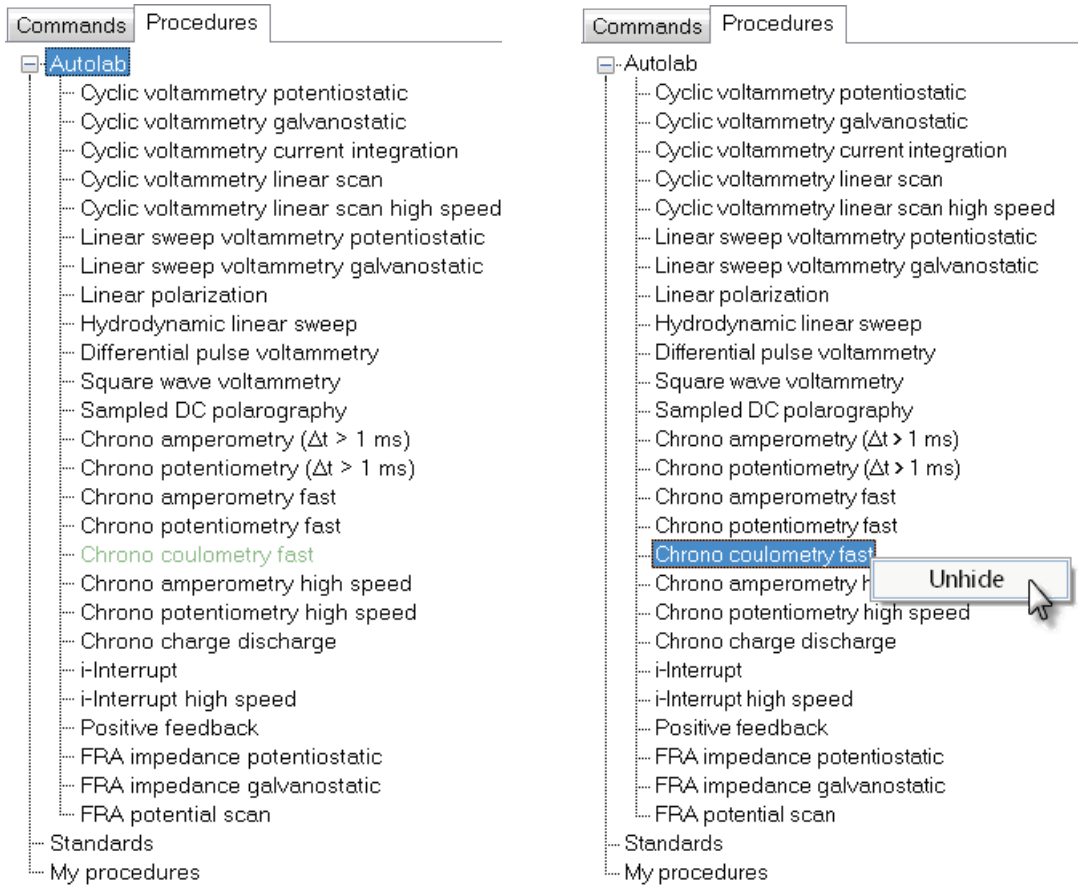


Figure 34 – Right click hidden items to unhide them

To unhide a hidden item, right-click the item and select the unhide option from the context menu, as shown in Figure 34.

Note: it is also possible to hide items using the CTRL-H keyboard shortcut and to unhide items using the CTRL-SHIFT-H keyboard shortcut.

In the commands browser, it is possible to hide single commands from a given group, using the same method. It is however also possible to completely hide a command group from the browser (see Figure 35).

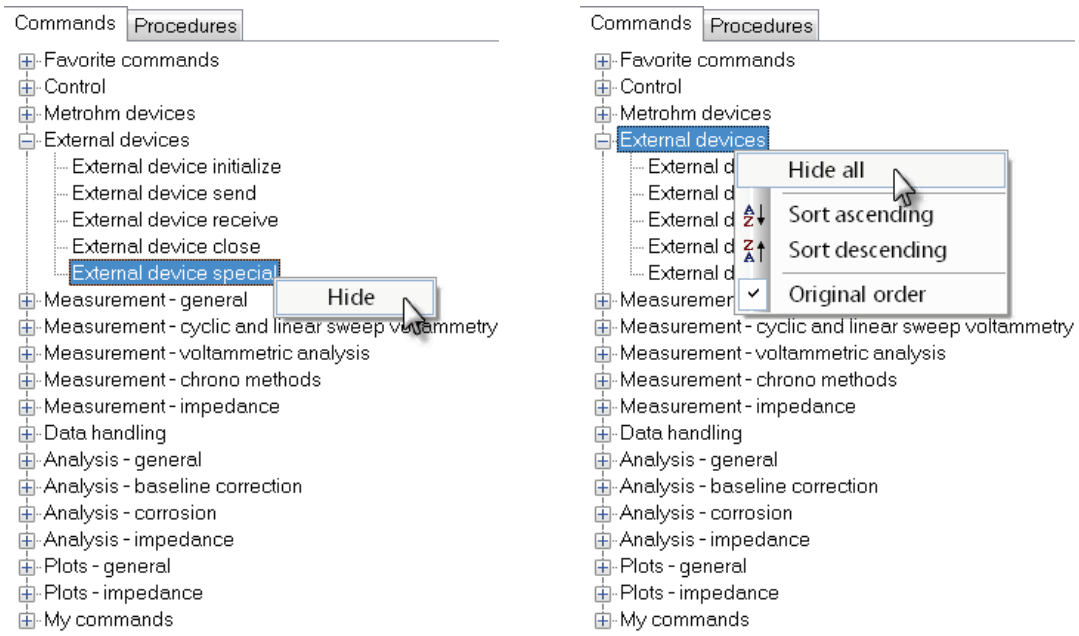


Figure 35 – Hiding a command (left) and a command group (right)

When a command group is hidden, the whole group will become invisible.

Finally, in the procedure editor, it is possible to hide or unhide command parameters, using the same method (see Figure 36). For example, if the interval time is not important, it can be hidden from view. This can be used to further simplify the user interface.

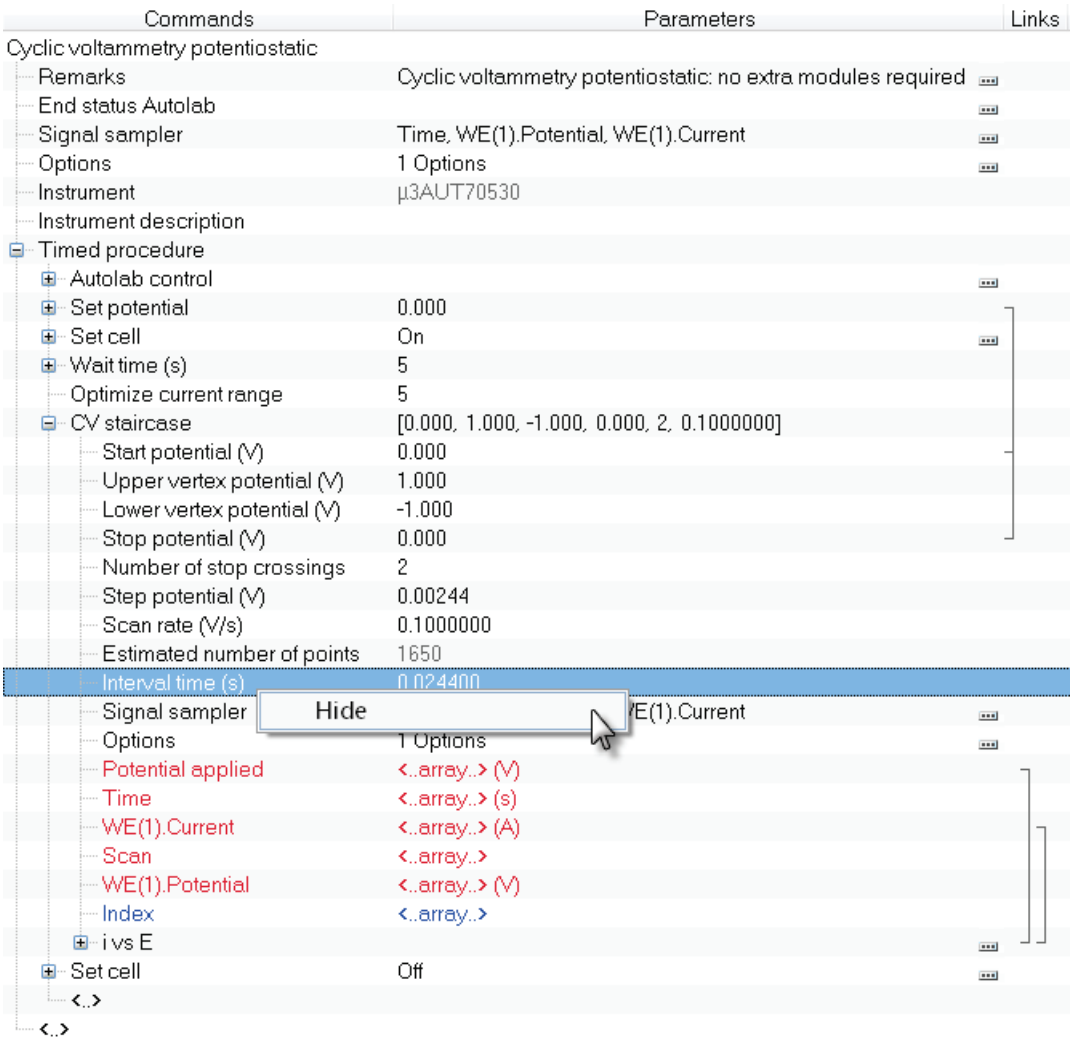


Figure 36 – Hiding and unhiding command parameters in the procedure editor

Sorting function for the commands browser

The possibility to sort the commands in a group is now provided. Right-clicking a command group displays the different sorting options: ascending or descending (see Figure 37). It is always possible to return to the original order using the same strategy and using the Original order option provided in the context menu.

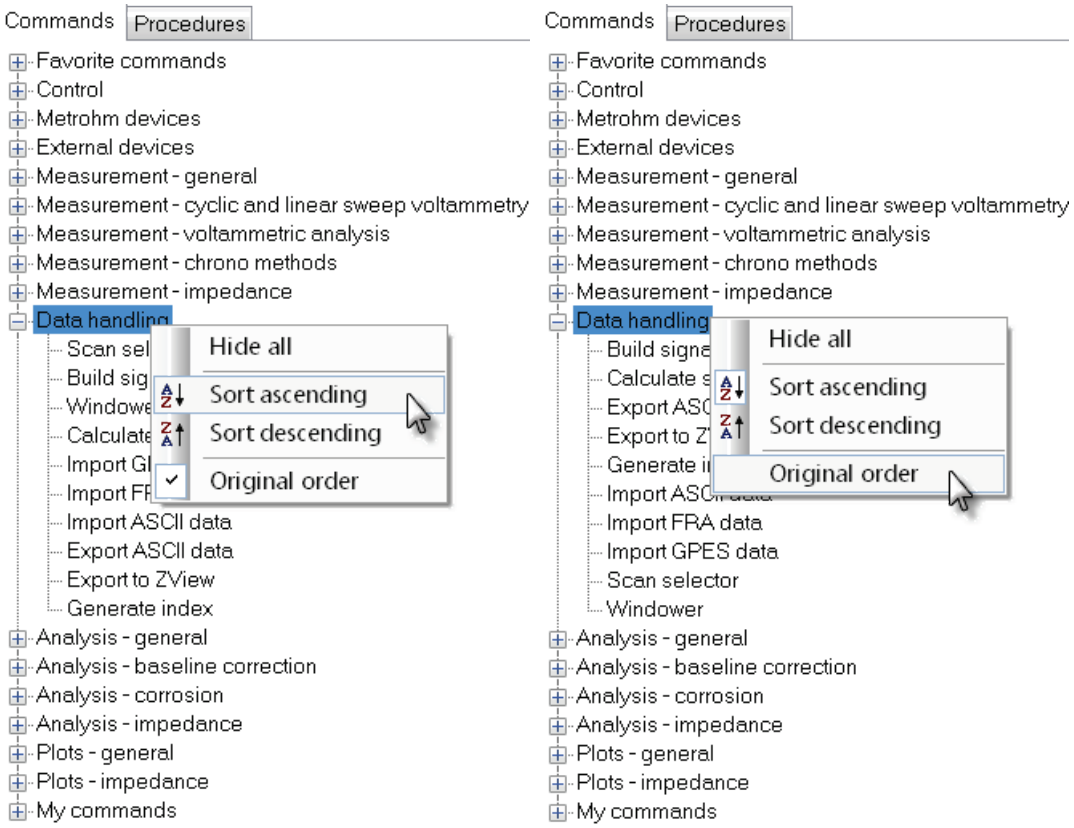


Figure 37 – Sorting the commands in a group in the commands browser

Import/Export profiles

It is possible to hide any number of items in Nova and to create a new profile for this customized view. Using the Profile menu, it is possible to import and export user profiles (see Figure 38).

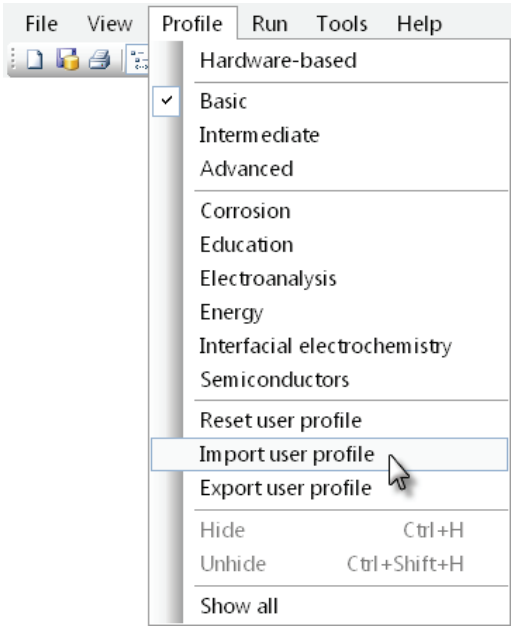


Figure 38 – Importing and exporting user profiles

This means that any number of profiles can be created and used at any time using this method.

It is possible to reset the user-defined profiles to default by using the Reset user profile option from the Profile menu (Figure 38).

Context sensitive popup menu

A new context sensitive popup menu window has been added to Nova. This popup appears as soon as any item supporting this feature is clicked (see Figure 39).

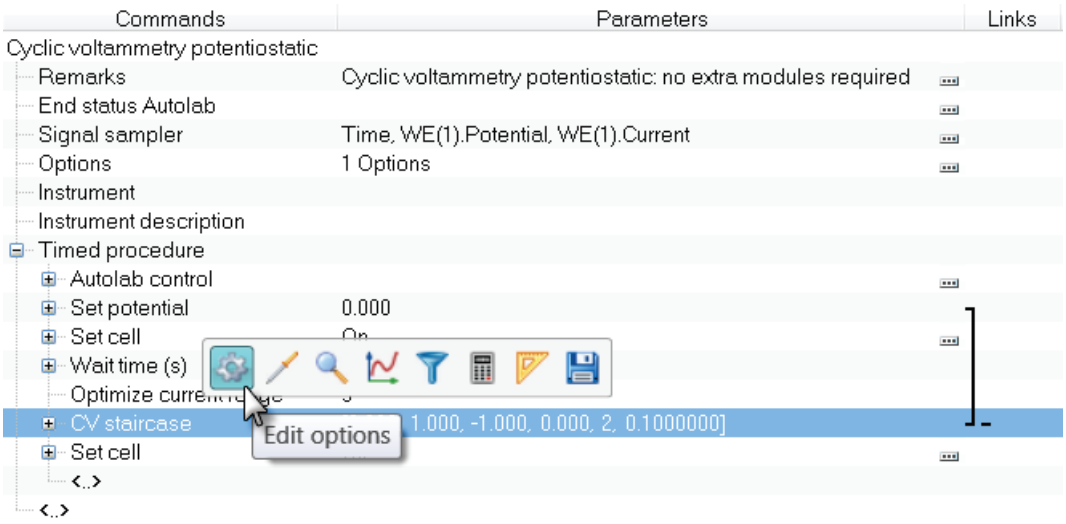


Figure 39 – Clicking an item in Nova now displays a popup menu window (for supported items only)

This popup menu displays a number of icons related to context sensitive actions. In the example shown in Figure 39, a total of eight action buttons are shown in the popup menu. These actions are the most commonly encountered for the CV staircase command (see Figure 40).

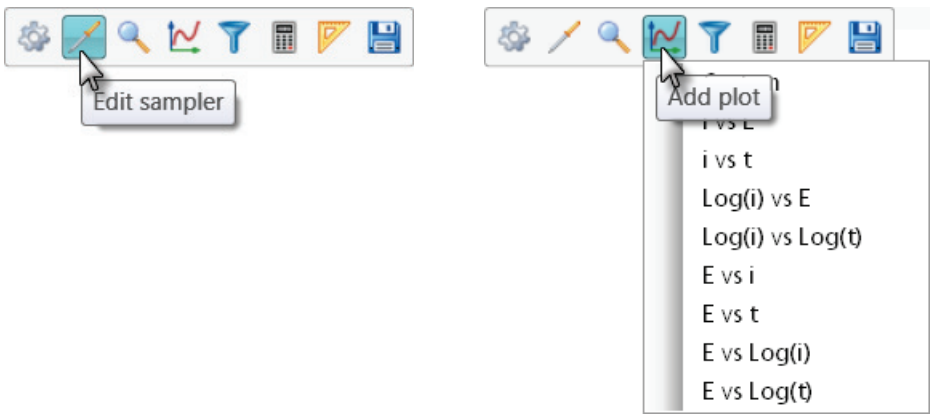


Figure 40 – Each icon in the popup menu is assigned to a specific action

This popup menu system can be used to facilitate procedure construction and data analysis.

Add comments to My commands

To simplify the organisation of commands saved in the My commands group, remarks can now be added to each command, as shown in Figure 64.

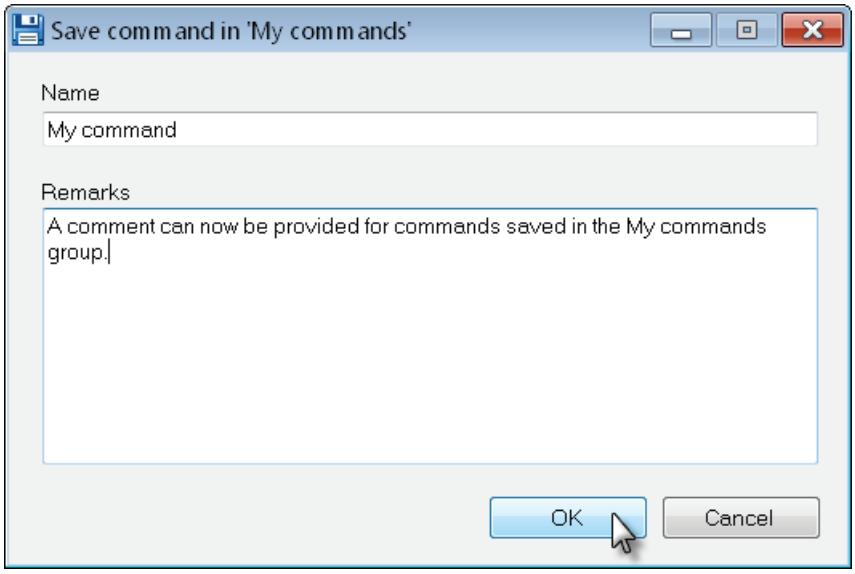


Figure 41 – Remarks can now be added to commands saved in the My commands group

The remarks provided upon saving the command are displayed in a tooltip in the commands browser (see Figure 42).

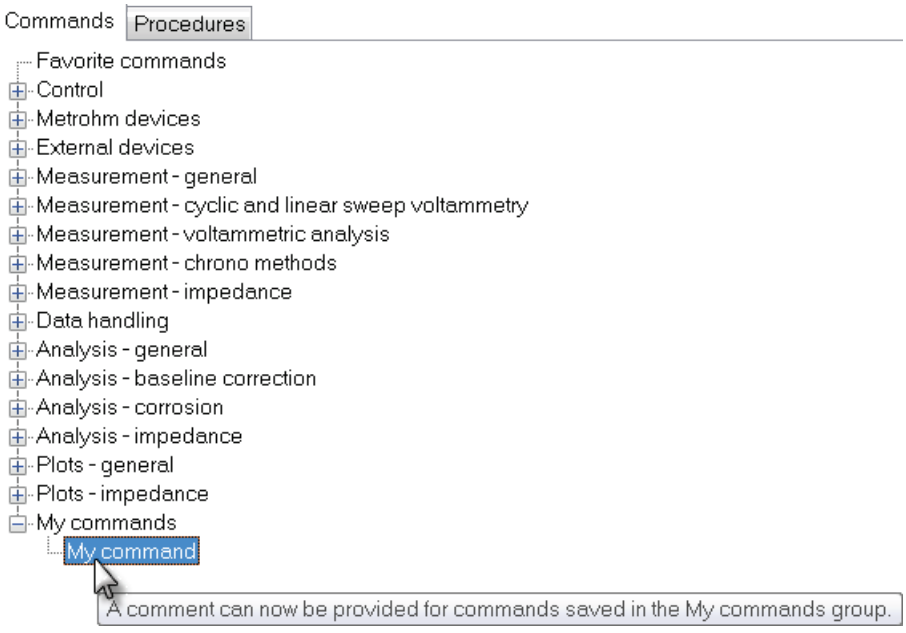


Figure 42 – The remarks are displayed in a tooltip for each command saved in the My commands group

Furthermore, it is possible to edit the remarks assigned to saved commands by right-clicking the commands in the My commands group (see Figure 43).

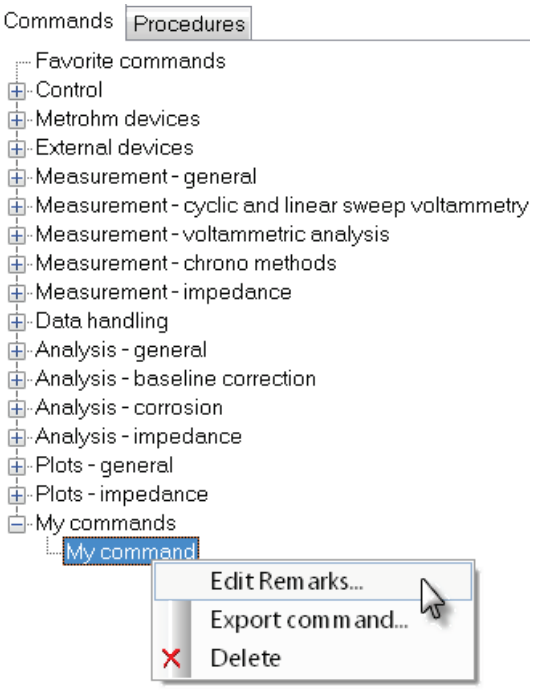


Figure 43 – Right click the commands saved in My commands group to edit the remarks

Favorite commands group

A new group, called Favorite commands, has been added to the Commands browser (see Figure 65).

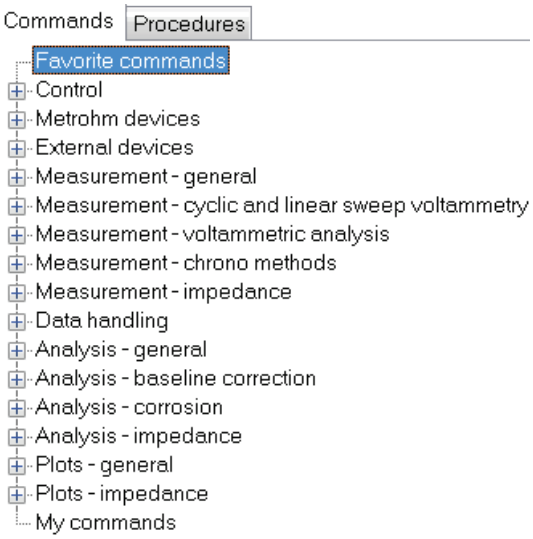


Figure 44 – A *Favorite commands* group has been added to the Commands browser

The Favorite commands group automatically displays the ten commands with the highest ranking (see Figure 45).

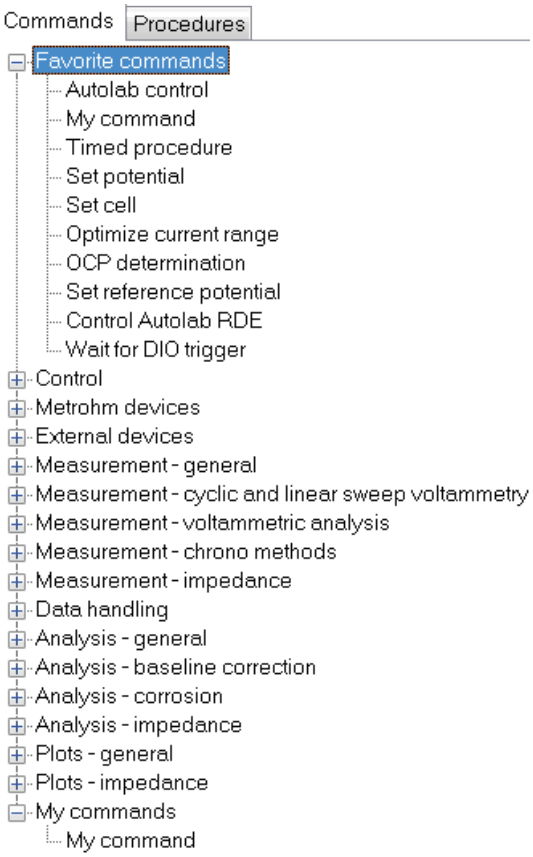


Figure 45 – The *Favorite commands* group displays the ten most used commands

User-defined commands, stored in the My commands group of commands, are also listed in the Favorite commands, if applicable.

It is possible to manually remove a command from the Favorite commands group by right-clicking the command (see Figure 46).

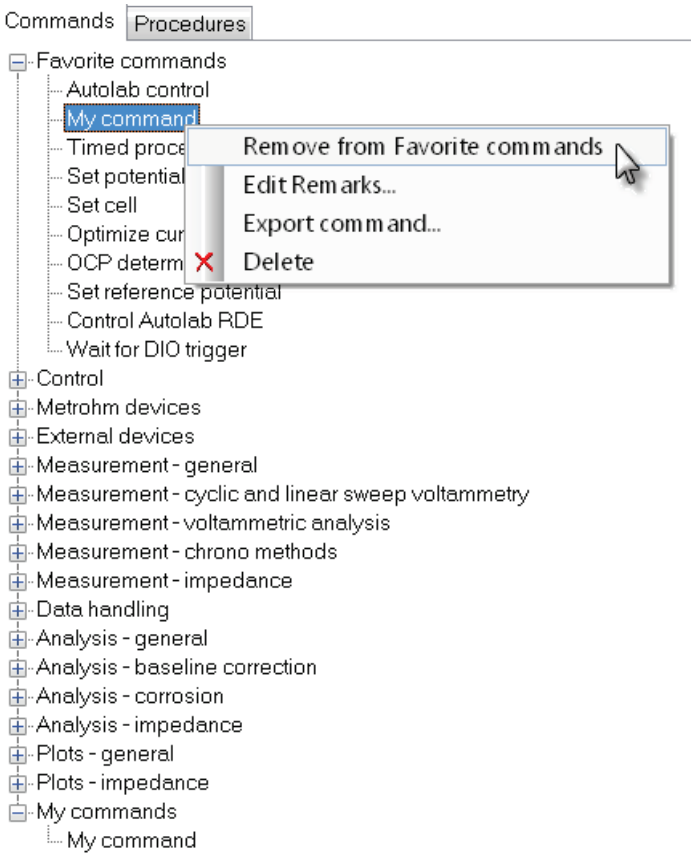


Figure 46 – Right click a command to remove it from the *Favorite commands* group

Manually removing a command from the list automatically forces the software to upgrade the 11th most used command to the favorite commands group.

Basic Undo/Redo functionality

The undo and redo functions have been added to Nova. The following actions can be undone or redone:

- Delete command
- Link or unlink command parameter
- Insert or move command

Note: command parameters have to be edited again in order to reset them to an earlier value.

Two buttons have been added to the toolbar (see Figure 47).

Figure 47 – The undo and redo buttons have been added to the toolbar

It is possible to undo an action by clicking the button in the toolbar if available or by right-clicking anywhere in the procedure editor (setup view) or the data explorer frame (analysis view) and select the **Undo …** option from the context

menu. In Figure 48 this tool is used to undo the delete action performed on the *CV staircase* command of the Cyclic Voltammetry potentiostatic procedure.

Note: the well known CTRL-Z keyboard shortcut can also be used.

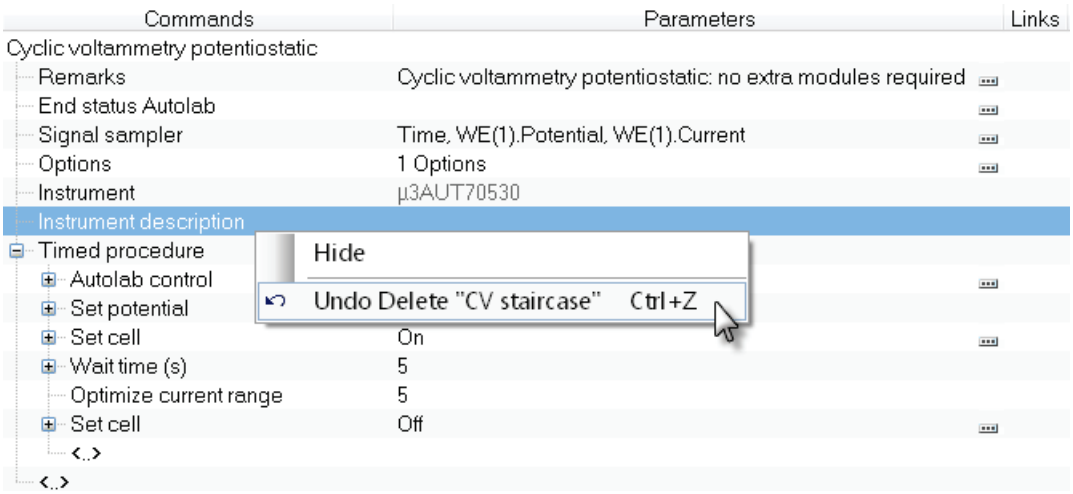


Figure 48 – Using the Undo function

Similarly, it is possible to redo an undone action by clicking the button in the toolbar or by right-clicking anywhere in the procedure editor (setup view) or the data explorer frame (analysis view) and select the **Redo …** option from the context menu. In Figure 49 this tool is used to redo the delete action performed on the *CV staircase* command of the Cyclic Voltammetry potentiostatic procedure.

Note: the well known CTRL-Y keyboard shortcut can also be used.

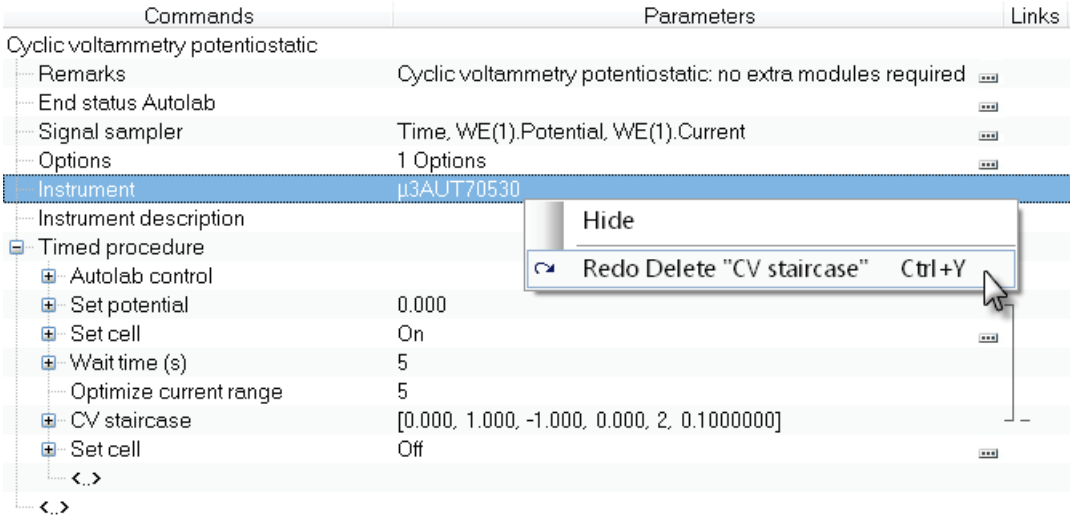


Figure 49 – Using the Redo function

Modification of the Calculate signal command

The *Calculate signal* command has been adjusted and now displays the expression used in the calculation in the procedure editor (see Figure 66).

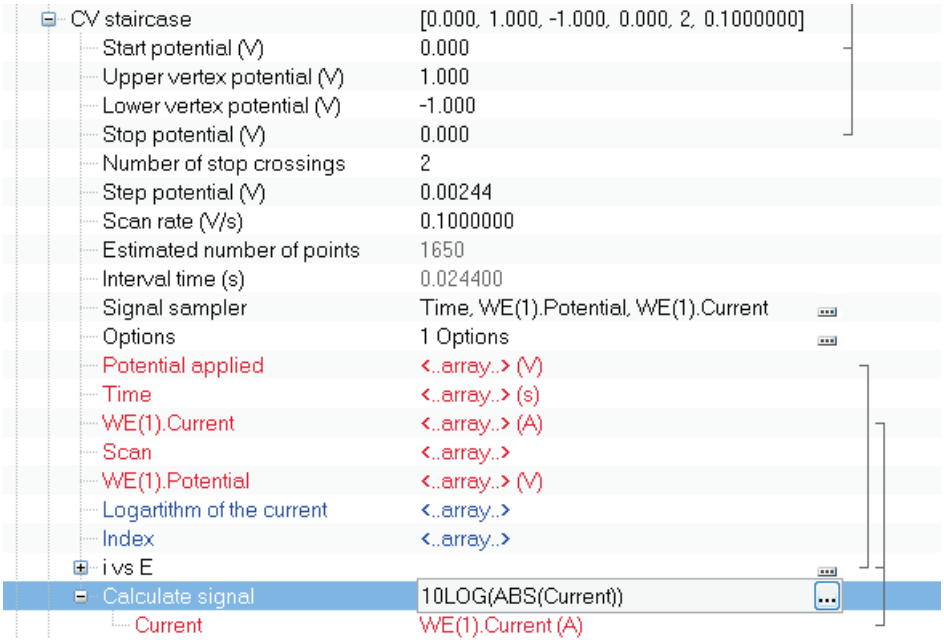


Figure 50 – The expression used in the *Calculate signal* command is now displayed in the procedure editor

Noise meters added to the Autolab display

A bar graph noise meter has been added to the Autolab display to indicate the level of noise recorded for both the potential and the current (see Figure 51).

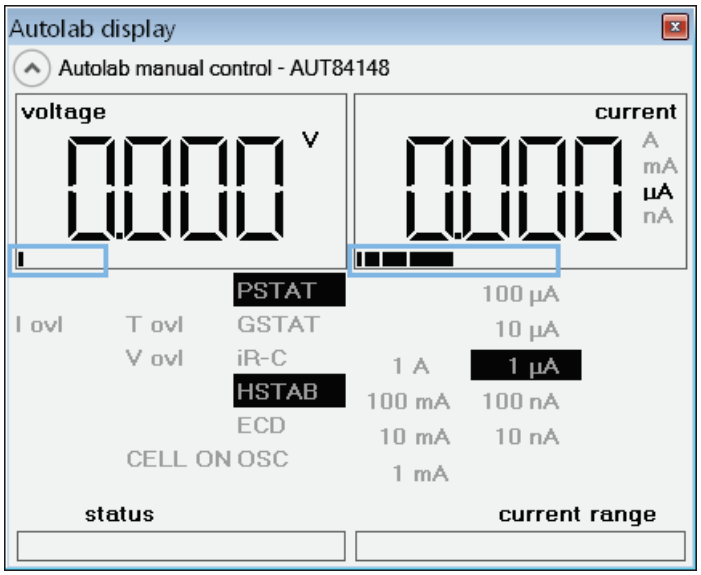


Figure 51 – Noise meters are now used to display the noise in the measurements

The noisier the signal, the more bars will be displayed. In Figure 51, the noise on the potential is very small (one bar), while the noise on the current is larger (four bars, out of maximum of eight).

Real time modification of the command parameters

It is now possible to modify certain command parameters while the measurement is running. In the measurement view, an additional frame is displayed during the experiment. If the running command offers the possibility to modify a parameter in real time, the current value will be displayed in the additional frame (see Figure 52).

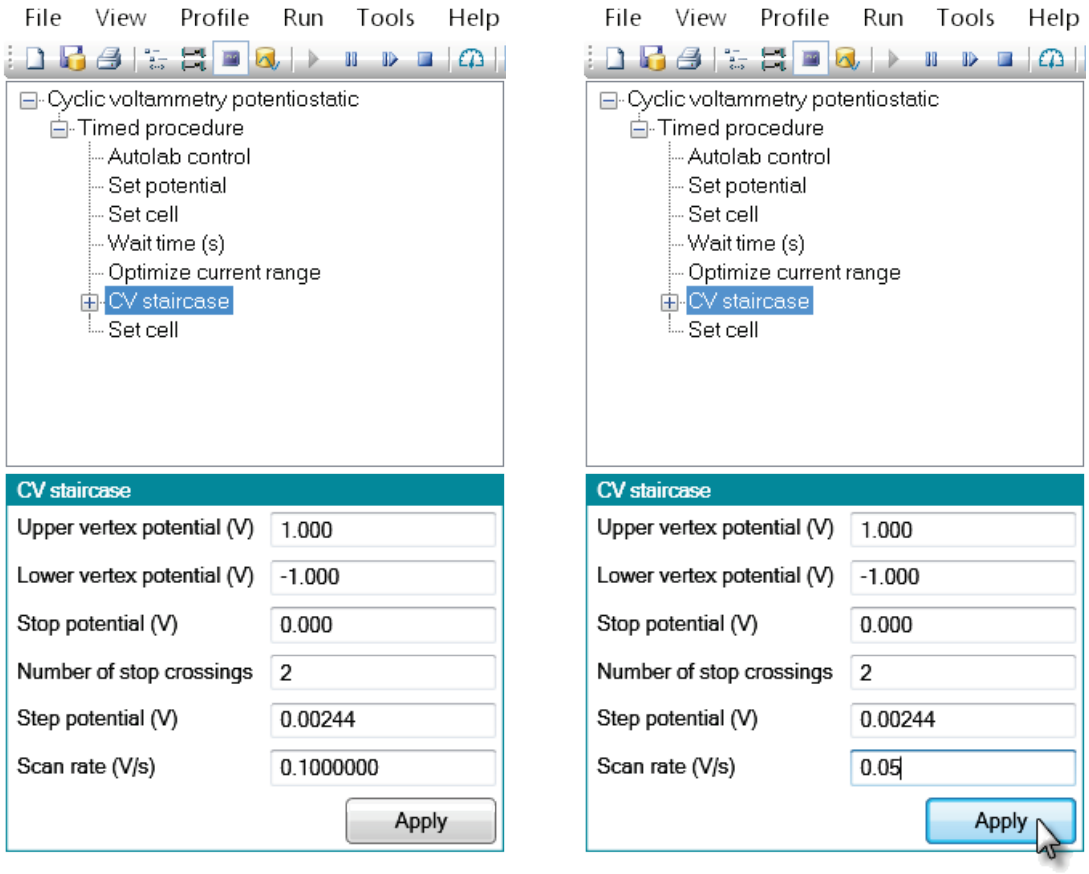


Figure 52 – The additional frame located in the measurement progress frame displays the list of modifiable command parameters (left: original parameters; right: modification of the scan rate)

In the example shown in Figure 52, the modifiable command parameters of the CV staircase command are displayed. To change a parameter, change the value and press the Apply button (see Figure 52).

Note: only the parameters of the active command can be modified. If the modified parameter is linked to other parameters in the procedure, the modification is applied to the linked parameters as well. The modification of the parameters only affects these parameters during the ongoing measurement. The original parameters defined in the procedure in the Setup view or not affected.

Add plots in real time

It is now possible to add new plots to a given command in the measurement view, while the command is running if the command provides data that can be plotted. Right-clicking the command in the measurement progress frame displays a context sensitive menu through which the type of plot and location can be chosen (see Figure 53).

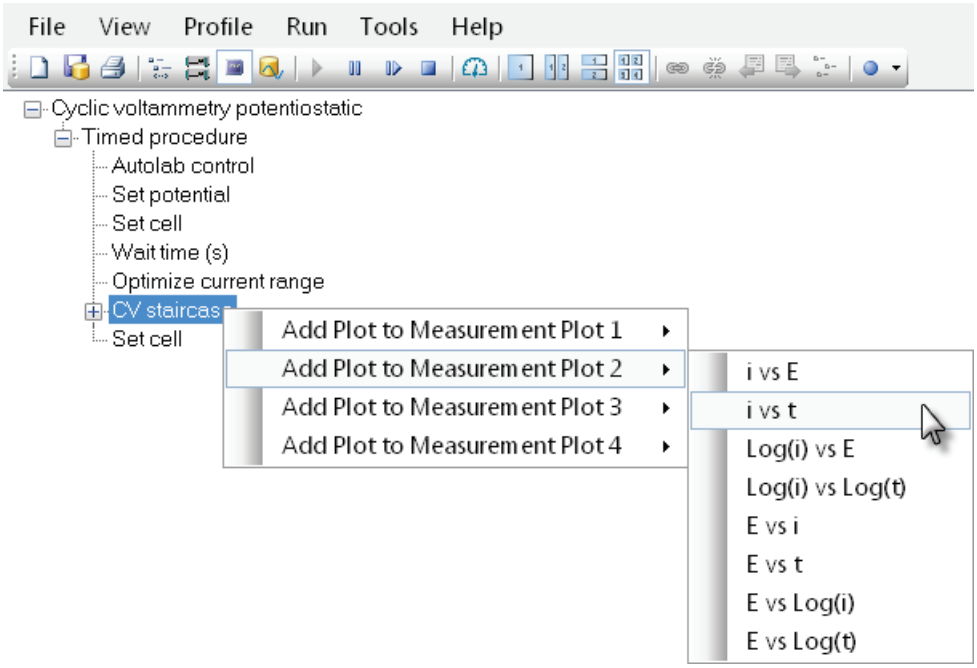


Figure 53 – Adding a plot to the CV staircase command

Note: the list of plots available in the right-click menu depends on the signals measured by the command. These signals are specified in the signal sampler.

Modification of the plot options in real time

It is now possible to change the plot options while the procedure is running. All the plots generated by a given command are now listed in the procedure progress frame. Right-clicking a plot displays a menu through which the plot options can be edited (see Figure 54).

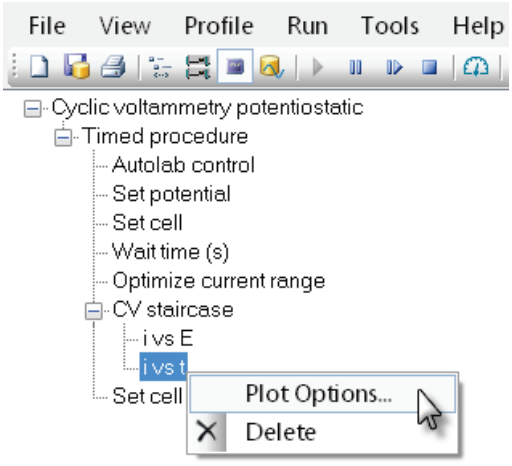


Figure 54 – It is possible to change the plot options while the measurement is running by right-clicking a plot in the measurement progress frame

Note: the same menu can be used to delete the plot (see Figure 54).

Create Windower from X axis

A new way of using the Windower tool has been added to the analysis view. It is possible to zoom in on the data shown in a plot to focus on a specific part of the plot (see Figure 55).

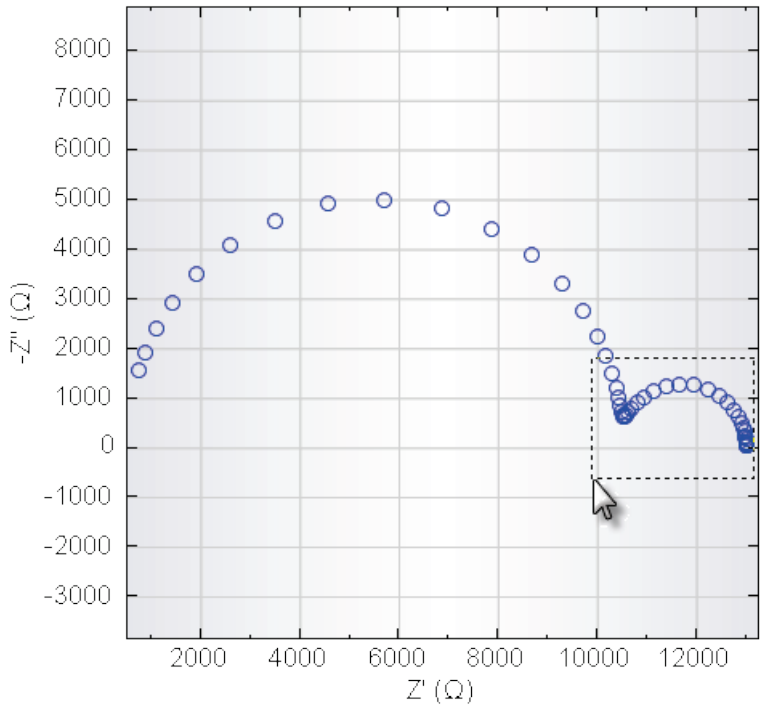


Figure 55 – Zoom in on the data

Next right click the plot in the data explorer frame and select the Create Windower from X axis option from the context menu (see Figure 56).

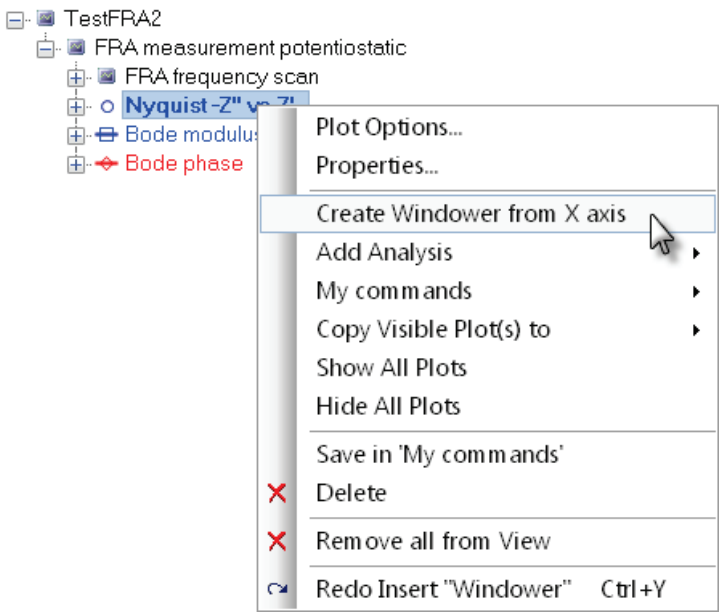


Figure 56 – Select the Create Windower from X axis option to window the visible data

The software will then add a Windower item to the data which will contain all the data that fit in the visible range of values for the signal plotted on the X axis. In the case shown in Figure 57, the Z' values between 9.8 kOhm and 13.2 kOhm have been windowed.

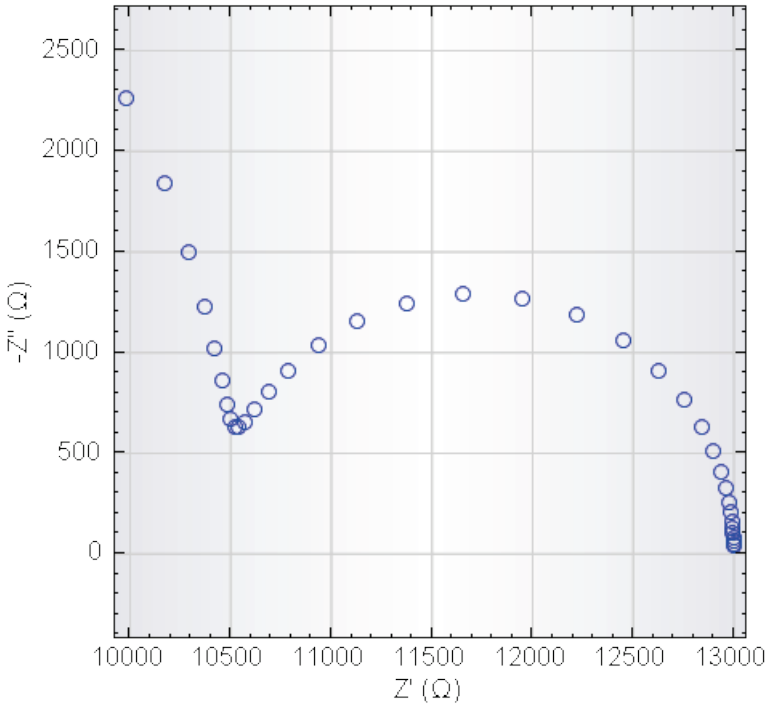


Figure 57 – The windowed data

New plot options

It is now possible to change the line plot and the combi plot in order to use a discontinued line instead of regular line (see Figure 58). Through a drop-down list, it is now possible to choose between different line styles.

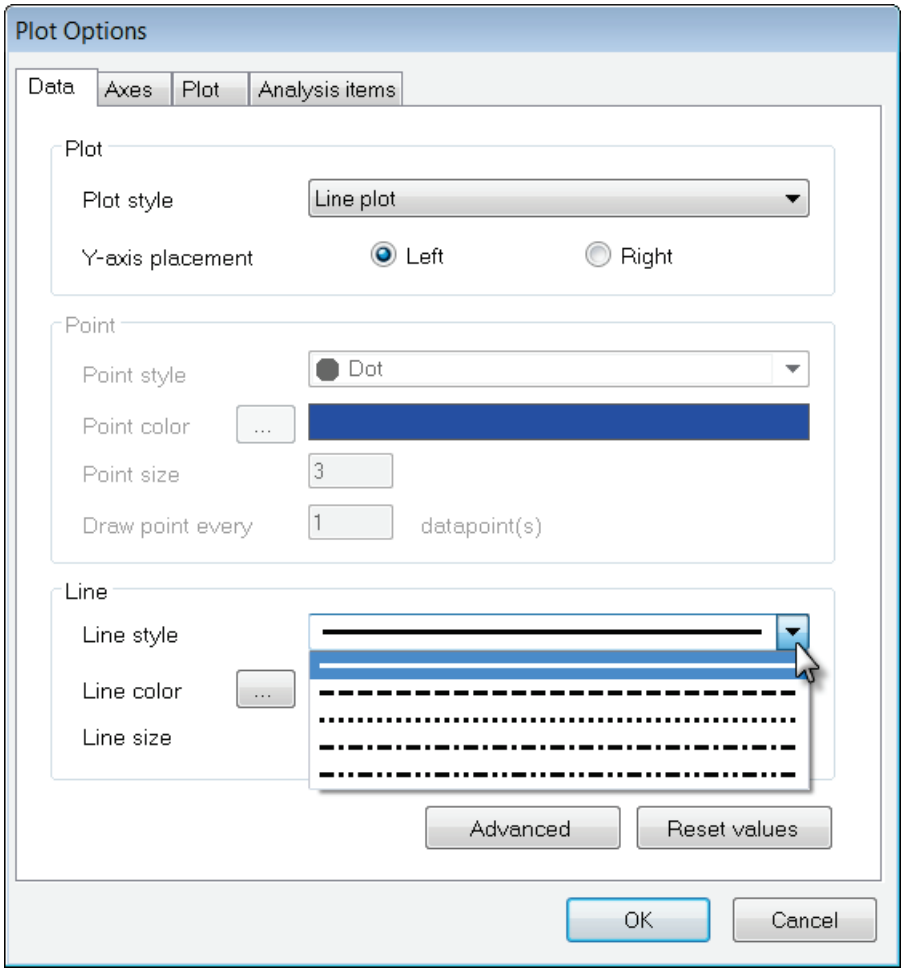


Figure 58 – A line style drop-down list has been added to the plot options

Linkable interval time in Record signal (> 1 ms) command

The interval time parameter of the *Record signals (> 1 ms)* command can now be linked to another parameter. The interval of the command can therefore be specified using an input box, for example (see Figure 74).

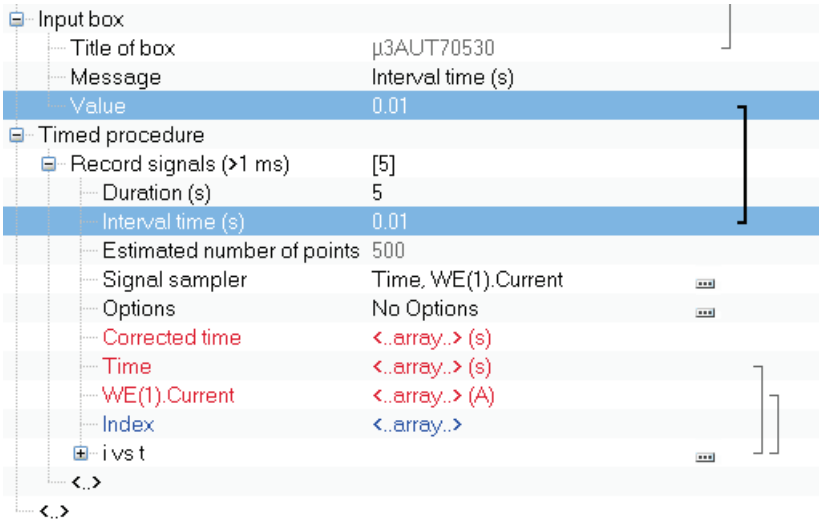


Figure 59 – The interval time parameter of the Record signals (> 1 ms) command is now linkable

Pseudo capacitance calculation for (RQ) circuit

The fitting and simulation tool for impedance spectroscopy now offers the possibility to convert a Q element in parallel with a resistance to a pseudo capacitance according to the following calculation:

$$C_{pseudo} = Y_0^{\frac{1}{n}} \cdot R^{\left(\frac{1}{n}-1\right)}$$

This option is shown in Figure 60. For example, a Q element with a Y_0 value of 1 µMho and a n factor of 0.75, in parallel with a resistance of 1000 Ohm will be converted to a pseudo capacitance of 51.8 nF.

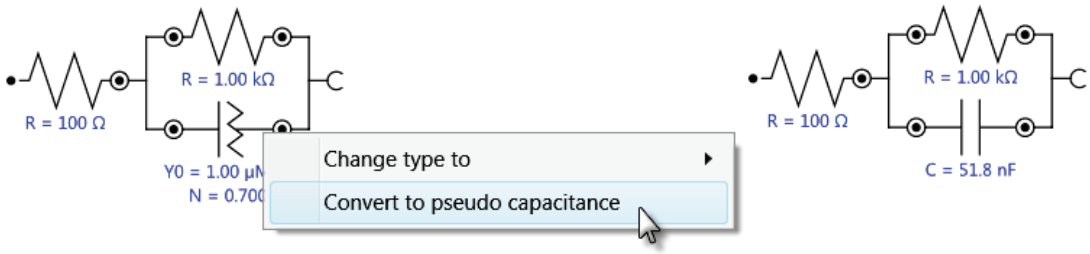


Figure 60 – Converting a Q element to a pseudo capacitance

NOVA 1.7 Release notes (Released 01/04/2011)

Introduction

These notes provide an overview of the new features introduced in NOVA 1.7 compared to the previous release.

The following items have been added to this release of NOVA:

- Support for the instruments and modules

  - PGSTAT302F – Switchable floating version of the PGSTAT302N
  - PGSTAT100N
  - Multi Autolab – Multi channel frame with M101 potentio-stat/galvanostat

- Improvements and additions

  - On the fly conversion of procedures and data from previous versions of NOVA
  - Redesign of the pX calibration interface
  - Redesign of Edit Cutoff user interface
  - Reverse on Cutoff
  - Adjustments to the Graphical user interface for Fitting and Simulation of impedance data
  - Improvement of the Peak search analysis tool
  - Driver manager
  - Export to ZView command
  - Integration of *My Commands* in Analysis view
  - Record signals linkable
  - Faster startup
  - Adjustments to the Windower tool
  - Preview of database names

Installation requirements

NOVA 1.7 requires the .NET Framework 4.0 to be installed. This windows update is automatically installed, if necessary, during the setup of NOVA 1.7 (see Figure 61).

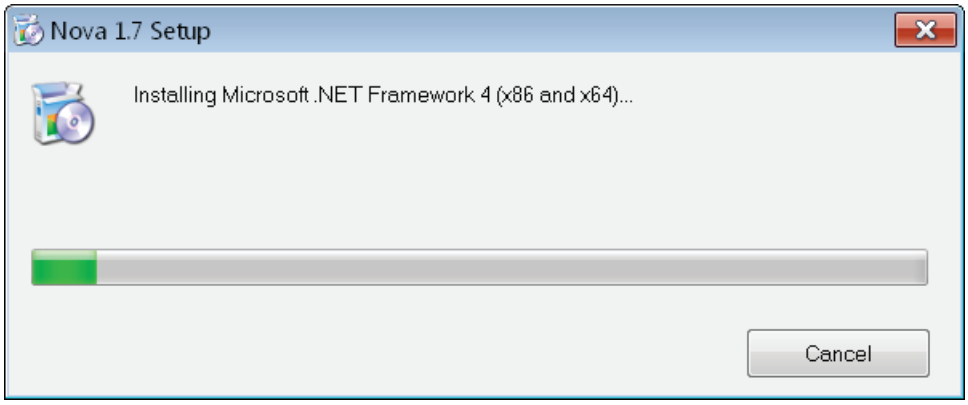


Figure 61 – NOVA 1.7 requires the .NET Framework 4.0

PGSTAT302F

The PGSTAT302F is a special version of the PGSTAT302N. This instrument can be toggled from normal operation mode to floating mode. The regular use is intended for typical electrochemical cells in which neither the working electrode nor the electrochemical cell itself are connected to ground. The floating mode is intended for grounded electrochemical cells or cells in which the working electrode is directly connected to ground.

Please note that the signal-to-noise ratio will deteriorate when working with the PGSTAT302F in floating mode. When the PGSTAT302F is operated in normal mode, the specifications will be identical to those of the PGSTAT302N.

More information on the PGSTAT302F can be found in the documentation provided with the instrument.

PGSTAT100N

The PGSTAT100N is the evolution to N-form factor of the Autolab PGSTAT100. It can now be selected in the Hardware setup.

Multi Autolab

The Multi Autolab is a generic frame in the same form factor as the PGSTAT302N. This frame can be fitted with additional modules (see Figure 62).

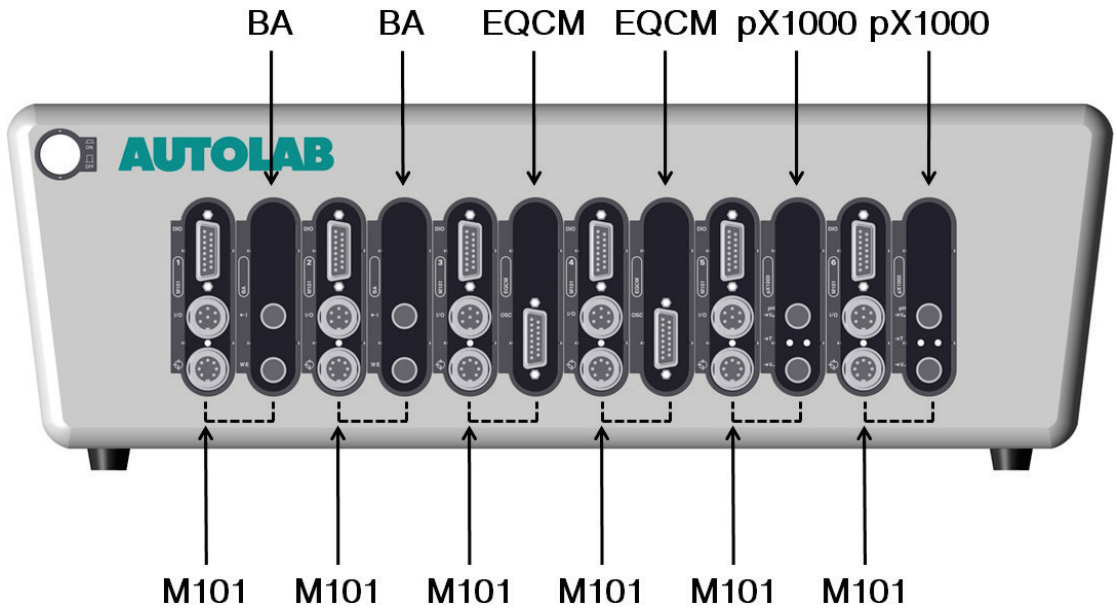


Figure 62 – Example of a Multi Autolab instrument fitted with M101 modules and daughter modules (BA, EQCM and pX1000)

The following modules can be installed in the frame:

- **M101:** this is a PGSTAT101 module, providing control for a single electrochemical cell. The specifications of the M101 module are identical to the specifications of the PGSTAT101. Up to 12 M101 modules can be installed in a Multi Autolab frame, providing connections for up to 12 independent electrochemical cells.
- **Daughter module:** it is possible to install an optional module in the module bay directly on the right hand side of a M101 module. The daughter module can only be installed in an even position (identified by a letter on the front panel). This means that every M101 module installed in an odd module bay in the Multi Autolab frame (identified by a number on the front panel) can control a single daughter module installed in the even position directly on the right. Any of the following modules can be installed in this position: BA, EQCM, pX1000 and MUX.

The M101 modules and optional daughter modules are used through the Multi Autolab view. Please refer to the Multi Autolab tutorial for more information.

Previous NOVA versions and NOVA 1.7

It is possible to install more than one version of the NOVA software on the same computer. Installing version 1.7 does not upgrade previously installed versions. However, it is only possible to use one version of the software at a time and data sets obtained with NOVA 1.7 cannot be used with previous versions of NOVA. The opposite situation is possible, using the conversion tool that is installed together with version 1.7, or by using the **Import data** and **Import procedure** tools available in the software (see Figure 63).

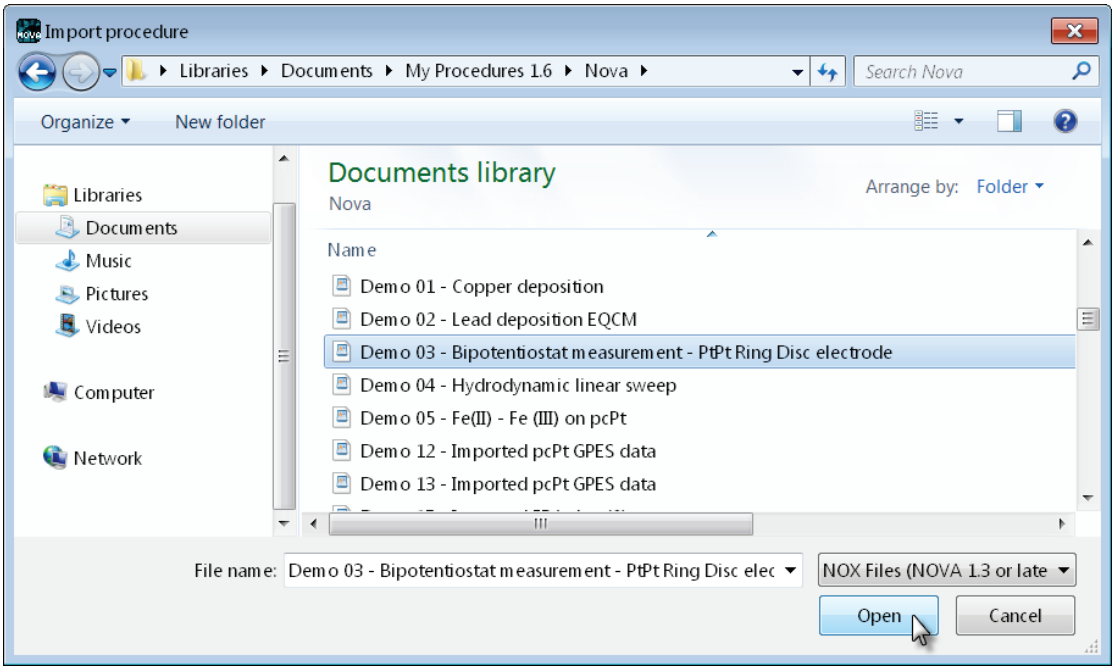


Figure 63 – It is now possible to import procedures and data from previous versions of Nova directly

Please refer to the **Upgrading files from previous versions** tutorial, available from the Help menu.

Note: files from NOVA 1.2 or earlier versions are no longer supported.

Redesign of the pH Calibration interface

The pH Calibration user interface has been redesigned for clarity. Redundant information has been removed and the calibration information is now displayed more clearly (see Figure 64).

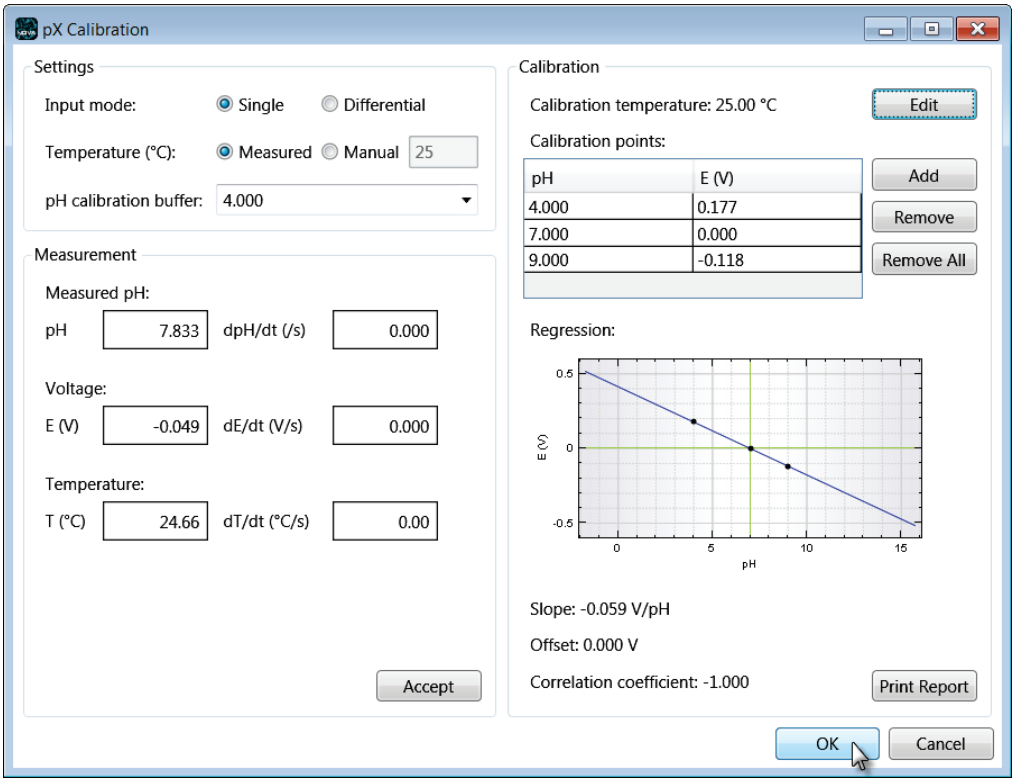


Figure 64 – The redesigned pH Calibration interface

The pH calibration tool requires the pX or the pX1000 module to be installed in the instrument.

Please refer to the pX tutorial, available from the Help menu in NOVA, for more information.

Redesign of the Edit Cutoff user interface

The Edit Cutoff user interface, integrated in the Edit Options menu, has been redesigned in order to present the cutoff definition in a clearer way with respect to the previous versions (see Figure 65).

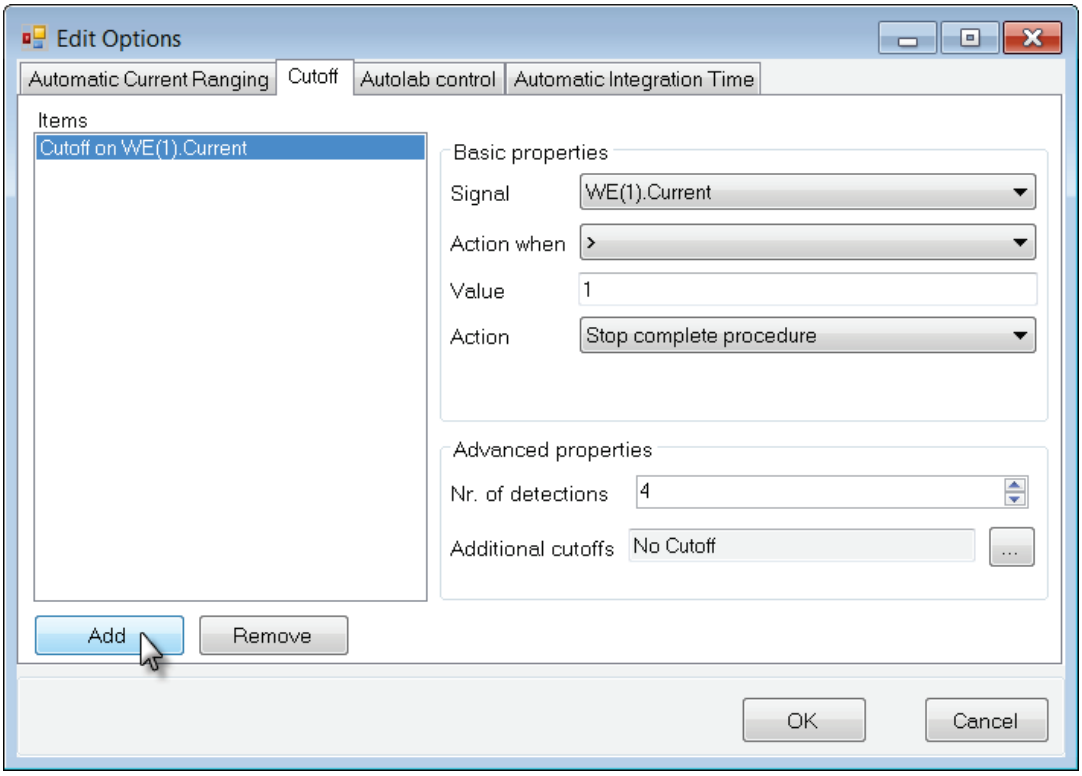


Figure 65 – The Cutoff user interface has been redesigned for clarity

Please refer to the Cutoff tutorial, available from the Help menu in NOVA, for more information.

Reverse on Cutoff

The redesign of the Edit Cutoff user interface now also includes a command specific action field which can be used to trigger a specific action when a user-defined cutoff condition is met during the execution of a specific command.

Presently, only the *CV staircase* and the *LSV staircase* commands make use of this option. For both commands, the possibility to trigger a reversal of the scan direction is provided. This **Reverse on cutoff** action is only available in the Edit Cutoff dialog specified for CV staircase and LSV staircase (see Figure 66).

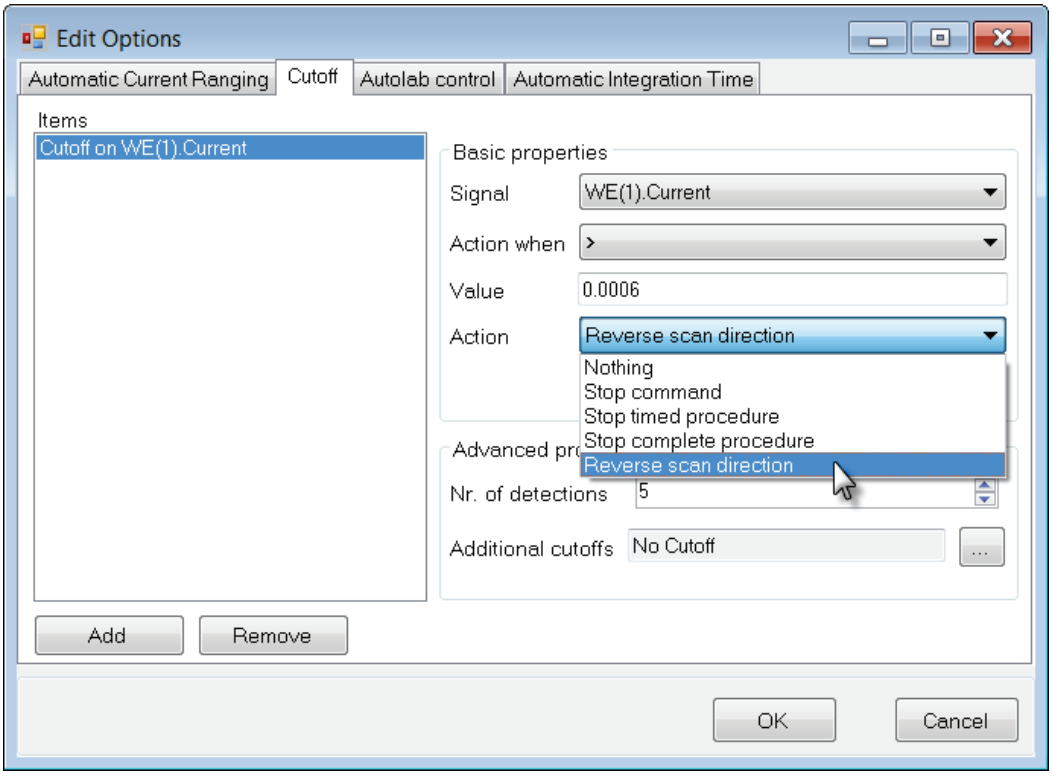


Figure 66 – The Reverse scan direction action can be specified in the cutoff for *CV staircase* and *LSV staircase* commands

Please refer to the Cutoff tutorial, available from the Help menu in NOVA, for more information.

Adjustments to the Graphical user interface for Fitting and Simulation of impedance data

The Graphical user interface for the fitting and simulation of impedance spectroscopy, introduced in NOVA 1.6, has been adjusted.

The following modifications are included in this release:

- **Unlinked connections are now identified in a unique way:** when connections in the graphical user interface are not combined properly in an equivalent circuit, they are indicated by an open circle (⊂) rather than a closed circle (○). This allows the user to identify the invalid connections more quickly (see Figure 67).

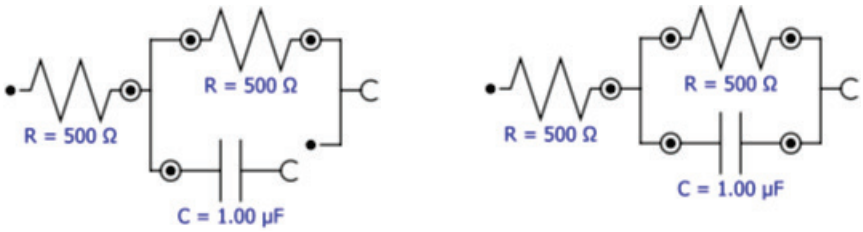


Figure 67 – Invalid connections are now indicated by an open circle (left, C element not connected properly; right, C element connected properly)

- **The χ^2 value is now included in the Report:** the calculated χ^2 value is now included in the report created by the Fit and Simulation tool (see Figure 68).

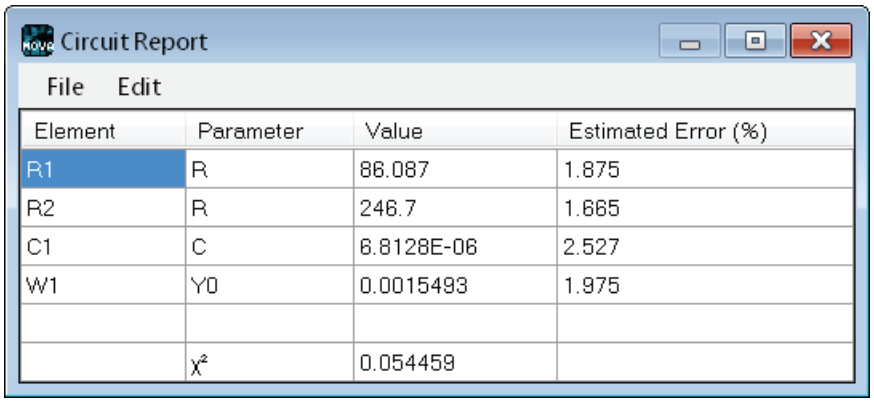


Figure 68 – The calculated χ^2 value is now automatically included in the report generated by the Fit and Simulation tool

Driver manager

The Autolab requires specific USB drivers in order to operate properly. Presently two different drivers are provided for the Autolab:

- **NOVA only driver (recommended):** this driver is only supported in NOVA. It provides faster USB data transfer with respect to the GPES drivers and provides support for up to 16 Autolab instruments connected to the same computer.
- **GPES compatible driver:** this driver is recommended for users that want to switch between NOVA and GPES. This driver provides slower data transfer and the maximum number of devices supported in Multi Autolab mode is 8.

It is possible to quickly switch between drivers by using the dedicated driver manager application. A shortcut is provided in Start menu – All programs – Autolab – Tools (see Figure 69).

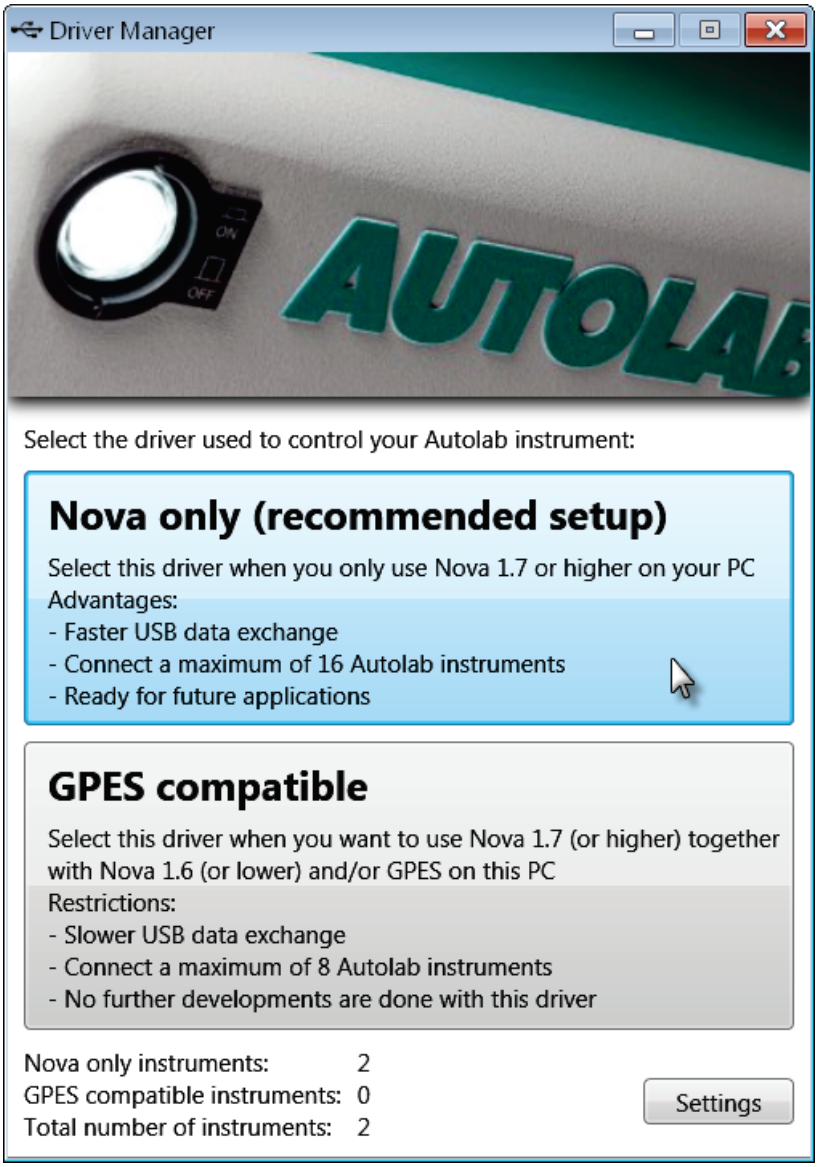

Driver Manager
AUTOLAB
Select the driver used to control your Autolab instrument:
Nova only (recommended setup)
Select this driver when you only use Nova 1.7 or higher on your PC
Advantages:
- Faster USB data exchange
- Connect a maximum of 16 Autolab instruments
- Ready for future applications
GPES compatible
Select this driver when you want to use Nova 1.7 (or higher) together with Nova 1.6 (or lower) and/or GPES on this PC
Restrictions:
- Slower USB data exchange
- Connect a maximum of 8 Autolab instruments
- No further developments are done with this driver
Nova only instruments: 2
GPES compatible instruments: 0
Total number of instruments: 2
Settings

Figure 69 – The Autolab Driver Manager application can be used to quickly switch from one driver to the other

The Autolab **NOVA only** driver is recommended.

Note: switch to the **GPES compatible** driver when using earlier versions of NOVA or when using the GPES or FRA software.

Improvements to the Peak search tool

The Peak search command and the corresponding analysis tool have been redesigned and improved. The parameter *Number of points in search window* is now defined in the Analysis view as a quick dial control (see Figure 70).

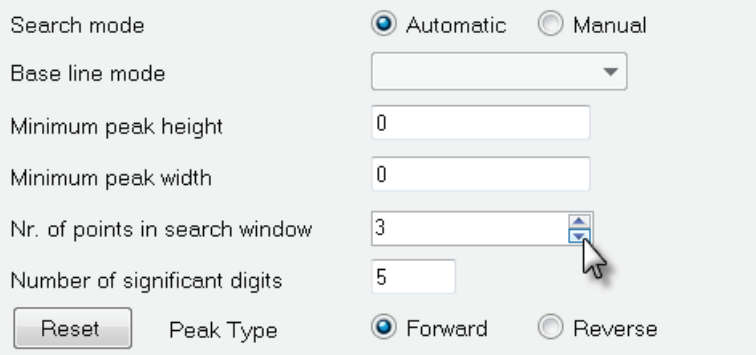


Figure 70 – The *Number of points in search window* parameter can now be adjusted with a quick dial

This allows the user to easily modify this parameter and visualize the changes in the peak search results. Moreover, the search algorithm is now also able to cross over data gaps. When encountering data sets with a gap, the peak baseline can be extended over the gap, if the gap distance is smaller than 3% of the X and Y value range (see Figure 71).

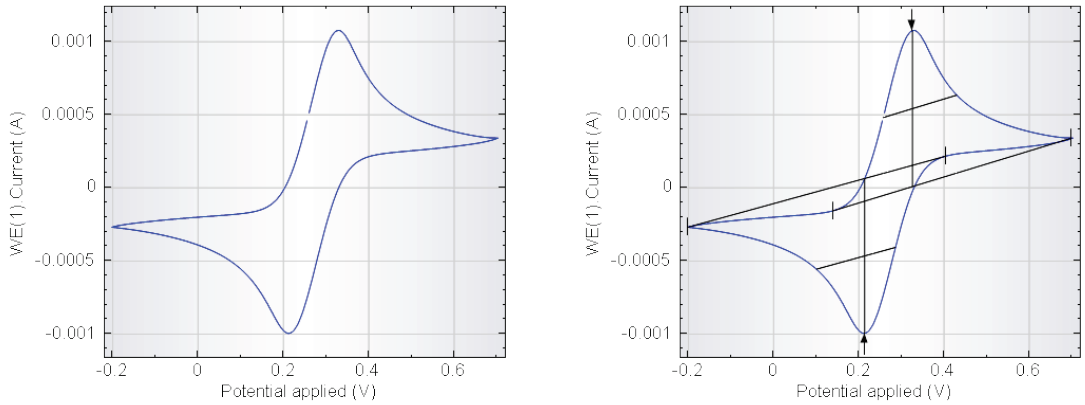


Figure 71 – The redesigned peak search tool is able to extend the baseline across data gaps (left, source data with gap around 0.25 V – right, result of peak search)

Export to ZView

A dedicated data exporting tool has been added to NOVA. Using this tool, it is possible to quickly export impedance spectroscopy data to a ZView compatible format (see Figure 72).

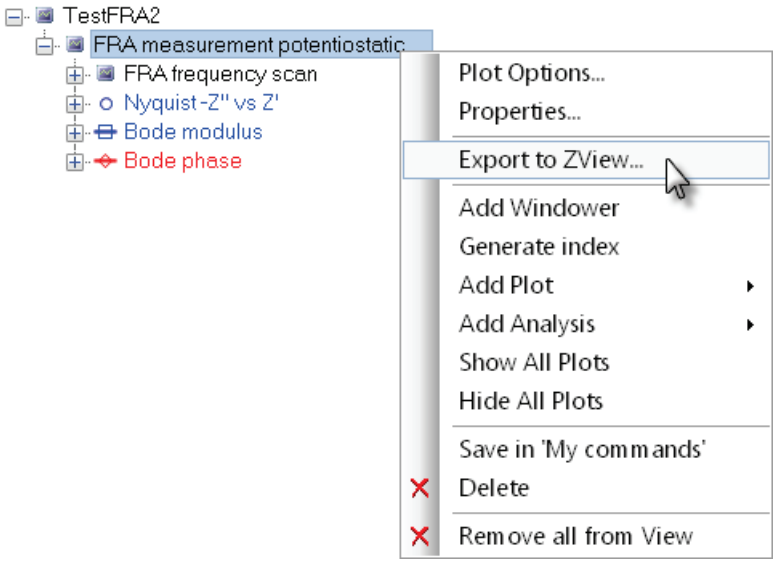


Figure 72 – A direct Export to ZView tool has been added

Using this tool, it is possible to create an ASCII file directly readable by the ZView software. A matching *Export to ZView* command has been added to the Data handling group of command in the Setup view.

My Commands integration in Analysis view

User defined commands created in the Setup view or in the Analysis view using the *My commands* framework can now be accessed from the Analysis view, using the right-click menu (see Figure 73).

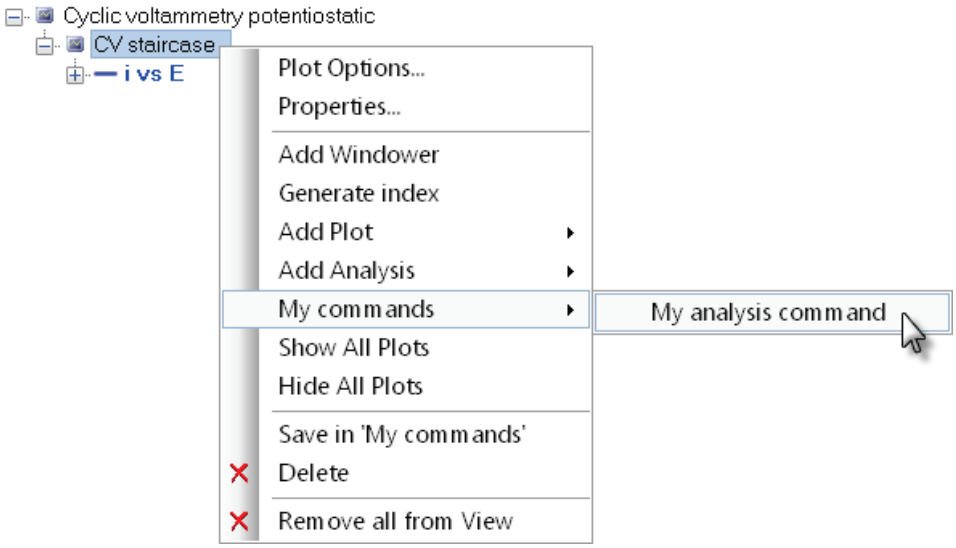


Figure 73 – Commands created using the *My commands* framework in the Setup view are now available in the Analysis view

Linkable duration in *Record signal (> 1 ms)* command

The Duration parameter of the Record signals (> 1 ms) command can now be linked to another parameter. The duration of the command can therefore be specified using an input box, for example (see Figure 74).

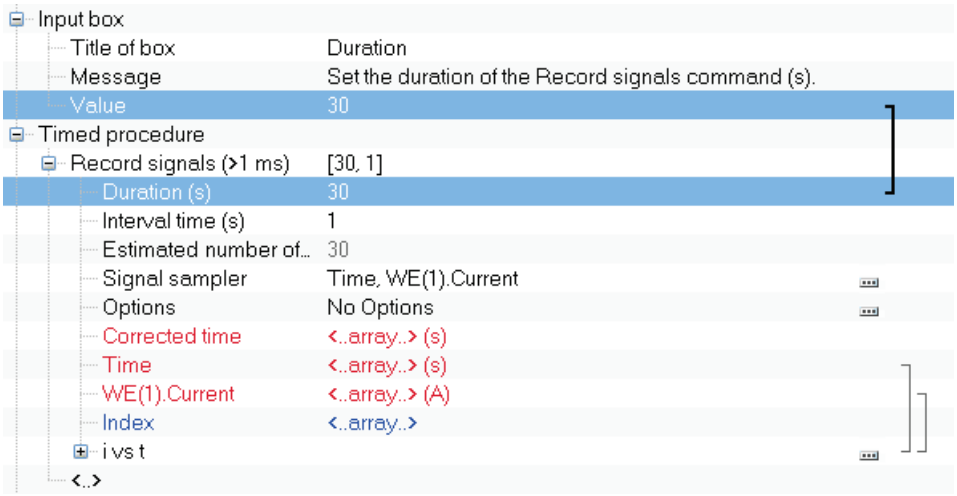


Figure 74 – The duration parameter of the Record signals (> 1 ms) command is now linkable

Faster startup of Nova

The boot sequence of the software has been improved with respect to the previous versions. Nova will now start considerably faster and the startup time is independent of the number of files in the database.

Adjustments to the Windower tool

The *Windower* command, available from the Data handling group, has been modified. The boundaries defined in the command can now be linked in the procedure editor to other parameters. The linkable boundaries are shown in the procedure editor after definition of initial values in the command (see Figure 75).

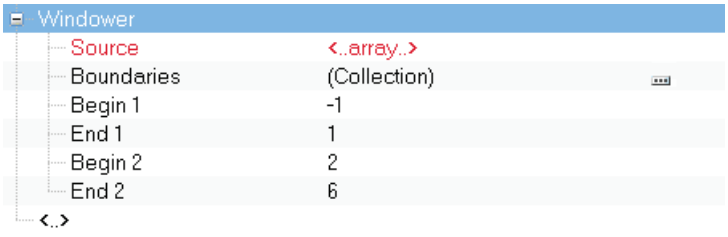


Figure 75 – The boundaries defined in the Windower tool are now available in the procedure editor

Preview of database names

When the Automatic save option is set to off (through the Tools – Options menu), the Save measured data dialog window will be displayed at the end of each measurement. To facilitate file naming, a drop-down list, displaying the list of files

already present in the database starting with the same name typed in the Procedure name field, is automatically generated (see Figure 76).

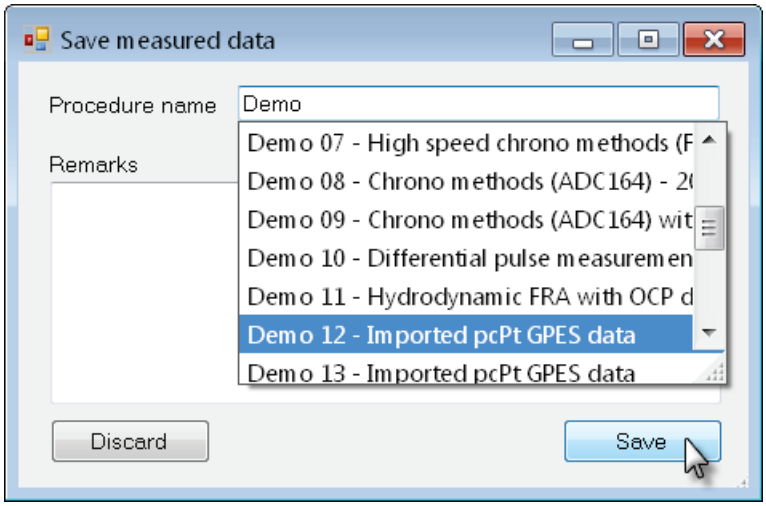

Save measured data
Procedure name
Demo
Remarks
Demo 07 - High speed chrono methods (F
Demo 08 - Chrono methods (ADC164) - 2
Demo 09 - Chrono methods (ADC164) wit
Demo 10 - Differential pulse measuremen
Demo 11 - Hydrodynamic FRA with OCP d
Demo 12 - Imported pcPt GPES data
Demo 13 - Imported pcPt GPES data
Discard
Save

Figure 76 – The Save measured data now automatically displays a list of file names already present in the database

NOVA 1.6 Release notes (Released 01/06/2010)

Introduction

These notes provide an overview of the new features introduced in NOVA 1.6 compared to the previous release.

The following items have been added to NOVA 1.6:

- A new set of tutorials, available from the Help menu

- Support for the modules

  - FI20 – Integrator and on-board integrator

- Improvements and additions

  - Serial number recognition
  - Redesign of the FRA measurement commands
  - Single frequency FRA measurements
  - Manual control of the FRA through Autolab display
  - Graphical user interface for Fitting and Simulation of impedance data
  - Simplified commands and parameters
  - MultiBA module support
  - Multi Autolab support
  - Software synchronization command for Multi Autolab measurements
  - Serial number and instrument description in the database
  - Multi Autolab support for Diagnostics application
  - New user interface for the procedure validator
  - FFT Analysis and FFT Smoothing
  - ECN Spectral noise analysis
  - Clear plot button modification
  - Dynamic command parameters
  - Repeat for multiple values
  - Autolab display with collapsible panels
  - Current interrupt and positive feedback
  - External .NET applications support
  - Avantes spectrometer support

Previous NOVA versions and NOVA 1.6

It is possible to install more than one version of the NOVA software on the same computer. Installing version 1.6 does not upgrade previously installed versions. However, it is not possible to use both software packages at the same time and data sets obtained with NOVA 1.6 cannot be used with previous versions of NOVA. The opposite situation is possible, using the conversion tool that is installed together with version 1.6.

Please refer to the **Upgrading files from previous versions** tutorial, available from the Help menu.

Tutorials

New tutorials have been added to this version of NOVA. The tutorials are available from the Help menu (see Figure 117).

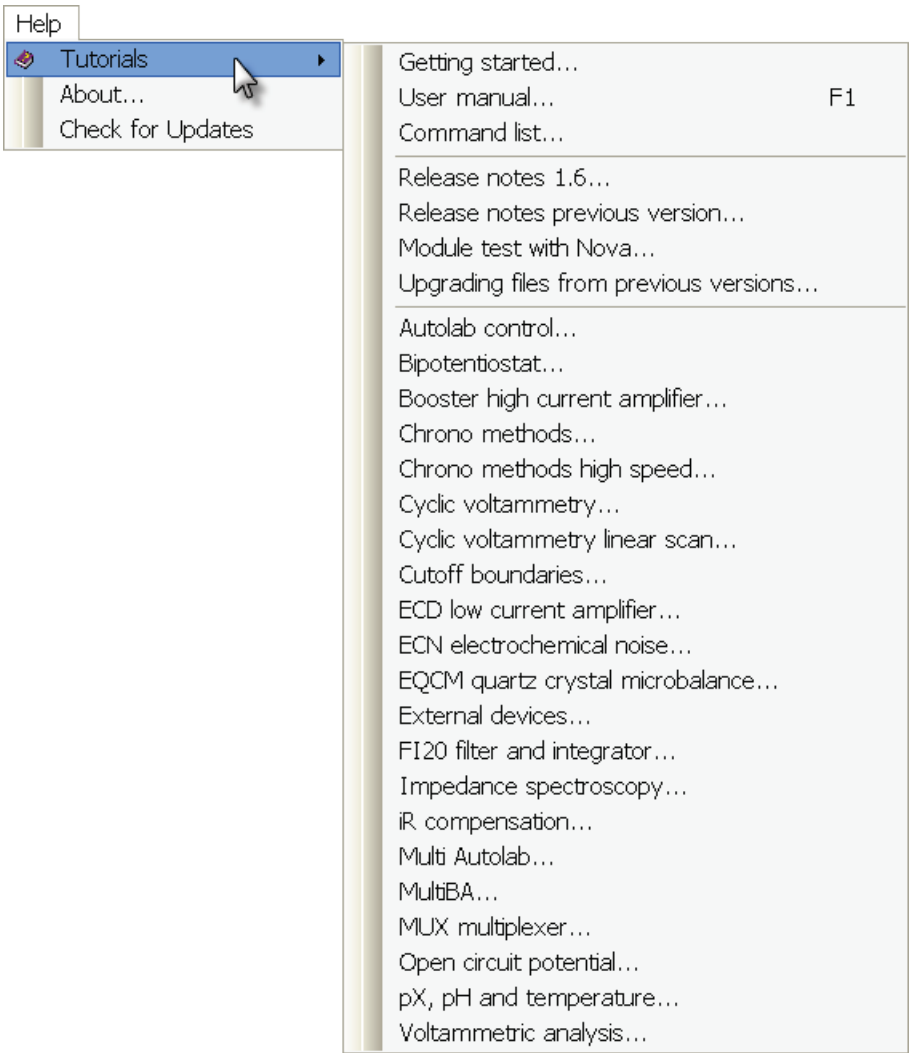


Figure 77 – New tutorials are available from the Help menu

Modules support

NOVA 1.6 adds support for the analog integrator part of the optional FI20 module. It also includes support for the on-board integrator of the µAutolab type II and III as well as the PGSTAT101 (see Figure 78).

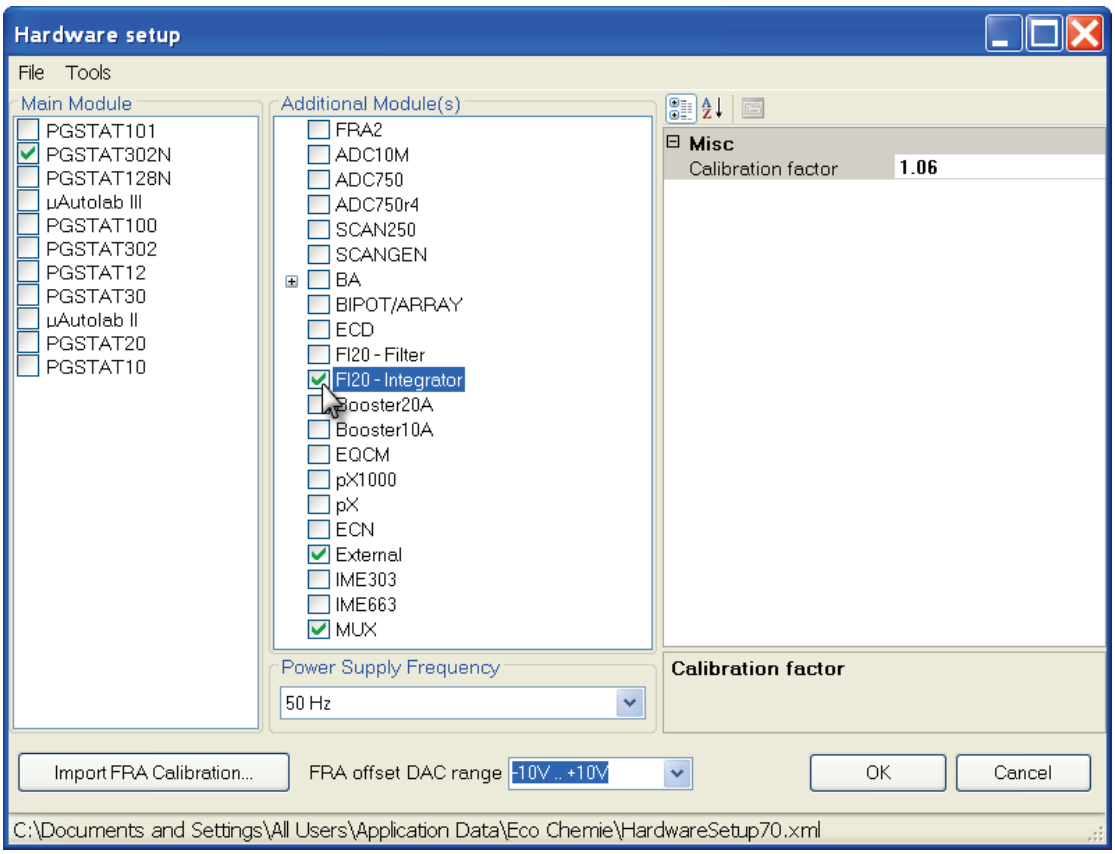


Figure 78 – The integrator module is now supported in NOVA

The integrator module can be used to measure the charge and perform chrono coulometry experiments. It can also be used to perform so-called Cyclic voltammetry staircase current integration experiments. Two default Autolab procedures have been added to illustrate the use of this module.

Warning: the integrator **must** be calibrated before it is used.

The calibration of the integrator is performed in the Diagnostics[4] application. Make sure that the **Integrator test** is selected in the diagnostics application (see Figure 79).

[4] Refer to the Getting started manual for more information on the Diagnostics application.

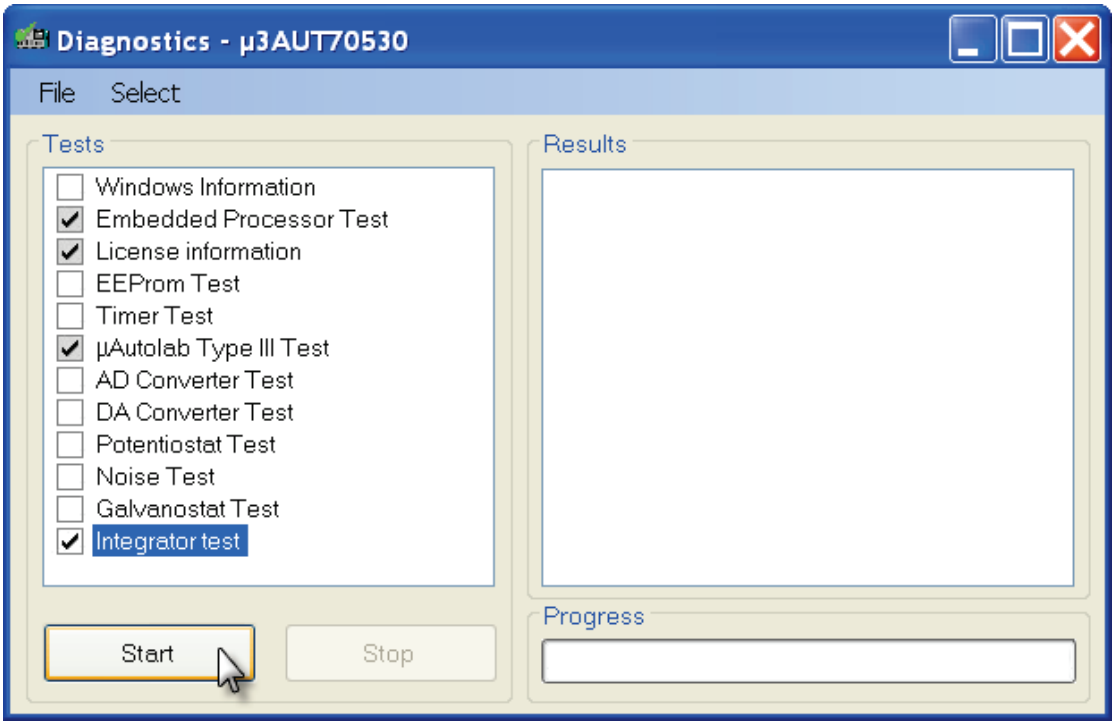


Figure 79 – The integrator test is used to determine the calibration factor of the integrator

When the integrator test is finished, a window will be shown, indicating the currently used calibration factor and the measured calibration factor (see Figure 80).

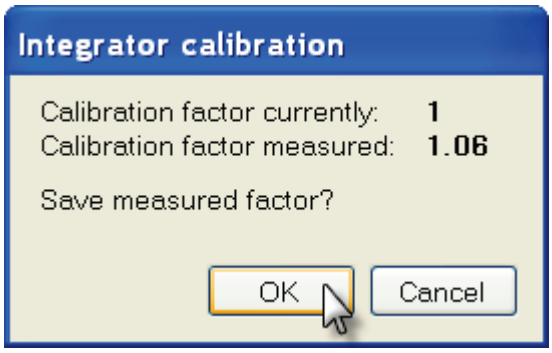


Figure 80 – The stored and measured calibration factors are shown at the end of the test

The new value can be stored by clicking the OK button. This value will be shown in the frame on the right-hand side of the Hardware setup window (see Figure 78).

More information on the use of the integrator module can be found in the **Filter and Integrator** tutorial, available from the Help menu.

Serial number recognition

Version 1.6 stores hardware setup profiles for each connected instrument. If the hardware setup is defined and saved on the computer for a specific instrument, this configuration file will be automatically loaded whenever the instrument is connected to the computer. The FRA2 calibration file is also associated with the identifying serial number of the device.

Note: it is not necessary to reboot the software whenever the hardware setup is adjusted.

Redesign of the FRA measurement commands

This version of NOVA includes a set of completely redesigned FRA measurement commands. The data acquisition speed has been significantly improved with respect to the previous versions of NOVA, without compromising data quality. Software overhead times have been reduced, resulting in a dramatic increase in data acquisition speed. The default Test FRA2 procedure provided in the Module test database will now take approximately four minutes instead of roughly ten minutes in the previous versions.

Through the added FRA sampler, time and frequency domain raw signals can be easily added to the measurement (see Figure 81). This additional information can be used to evaluate important experimental settings during measurement, like the linearity or the stability of the system being investigated.

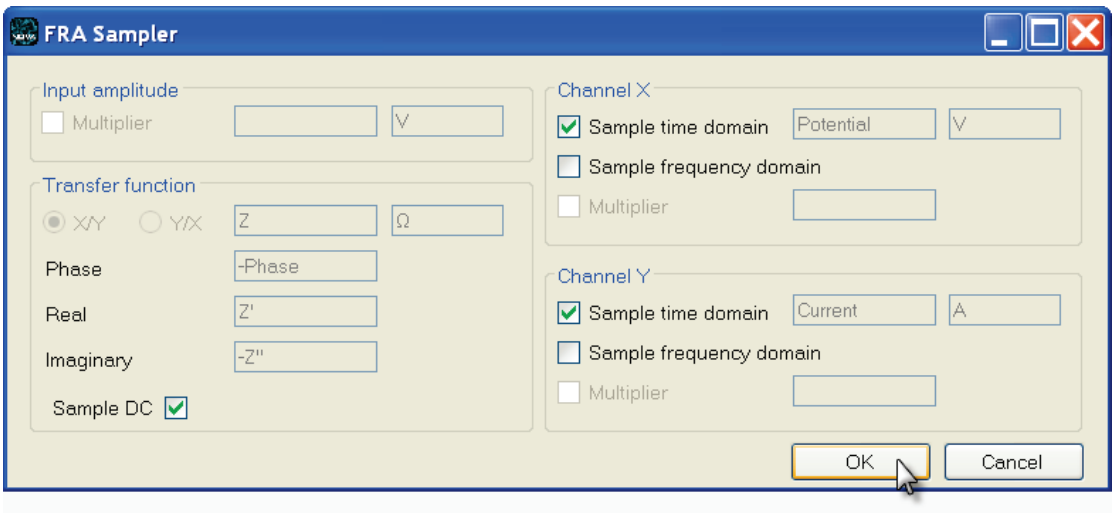


Figure 81 – The new FRA sampler can be used to sample time and frequency domain information during FRA measurements, as well as the dc components

The FRA related commands have been redesigned and the fundamental parameters of the FRA measurements can now be used in combination with other commands, using links.

For example, it is possible to define the amplitude to be used in the frequency scan, through an Input box or a calculation (see Figure 82).

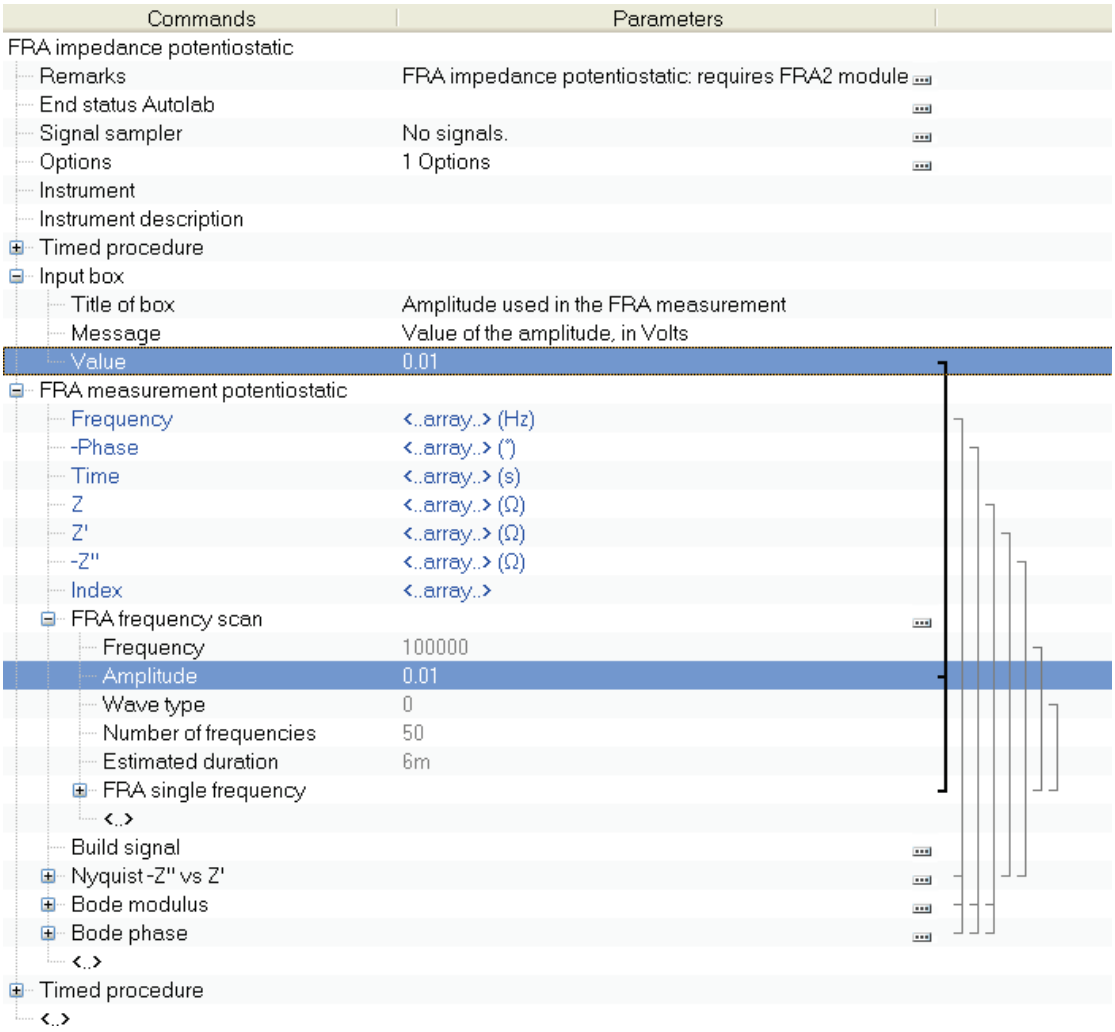


Figure 82 – Linking an Input box to the amplitude used in the FRA measurement

Single frequency measurements are now also possible as well as time scan FRA measurements. The Time signal is sampled for each impedance data point. This signal consists of the total elapsed time since the beginning of the experiment. This allows the user to track the progress of the measurement in long experiments or in time scan experiments.

Impedance measurements requiring connections to and from external devices are now easier to configure. The FRA sampler has been designed to allow the user to specify all the parameters of the external transfer function from one single location (see Figure 83).

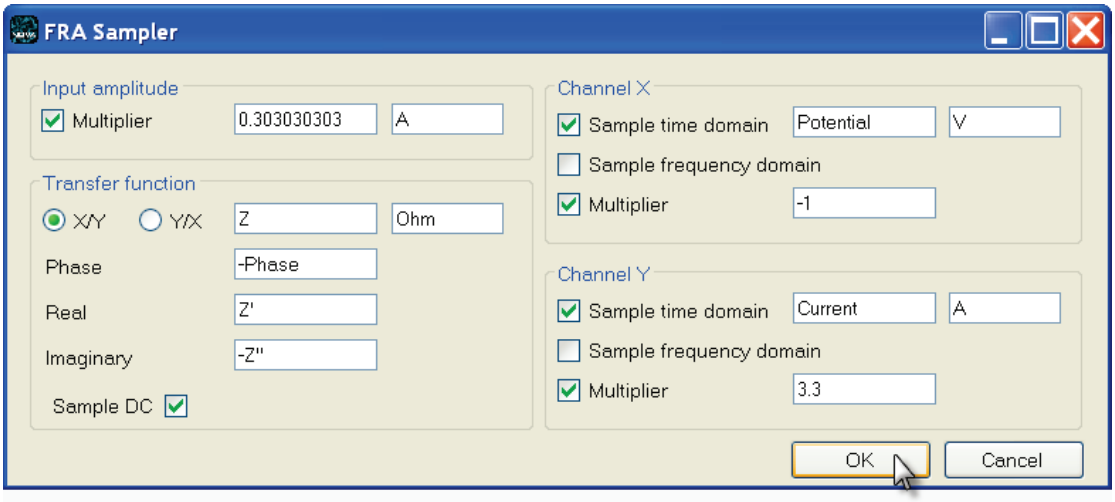


Figure 83 – The FRA sampler used for measurements in combination with a Kikusui PLZ164WA electronic load

The commands required for these measurements can be found in the Measurement – impedance group of commands and more information about impedance spectroscopy measurements can be found in the Impedance spectroscopy tutorial.

Single frequency FRA measurements

Using the *FRA single frequency* command, available from the Measurement – impedance group of commands, it is now possible to perform a single frequency measurement. It is not necessary to setup the complete *FRA frequency scan* command for this type of measurement (see Figure 84).

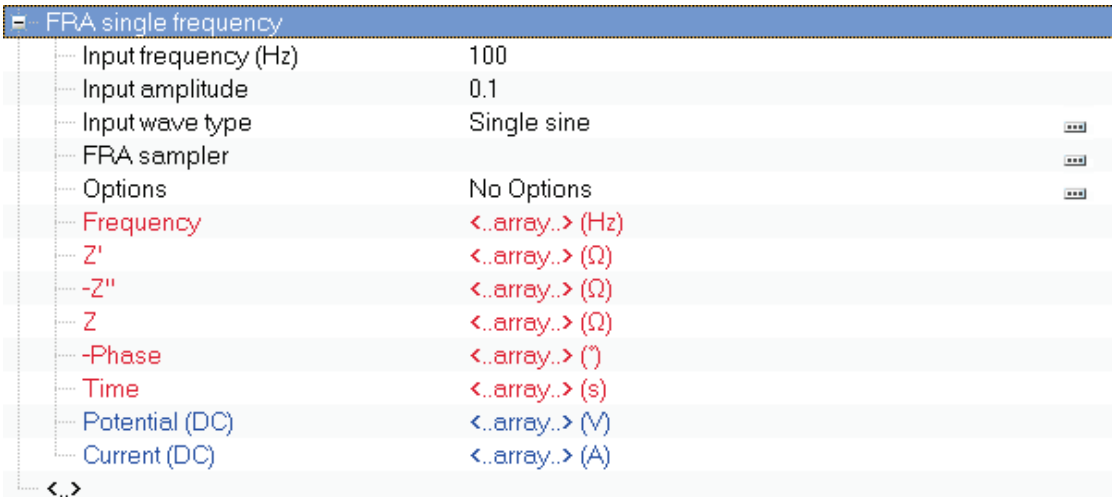


Figure 84 – Single frequency measurements are now possible using the *FRA single frequency* command

Manual control of the FRA through Autolab display

A panel system has been added to the Autolab display window. It is now possible to add or remove additional panels to this window, by picking the corresponding item in the view menu (see Figure 85).

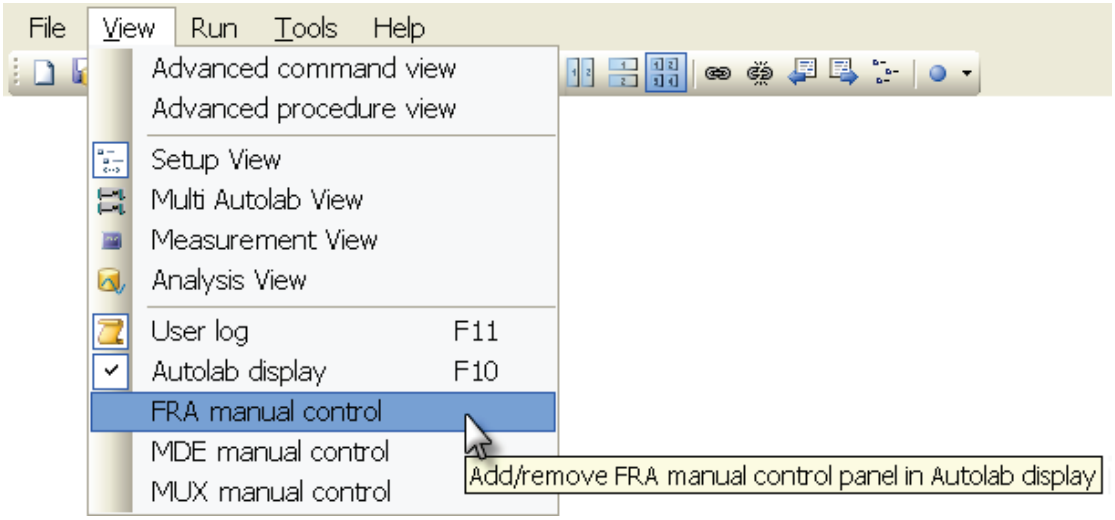


Figure 85 – Adding the FRA manual control panel to the Autolab display

When the *FRA manual control* option is selected, an additional panel will be available in the Autolab display window (see Figure 86). Using this panel, it is possible to perform manual measurements using the FRA2 module. The frequency and amplitude can be directly defined in the panel, as well as other relevant parameters.

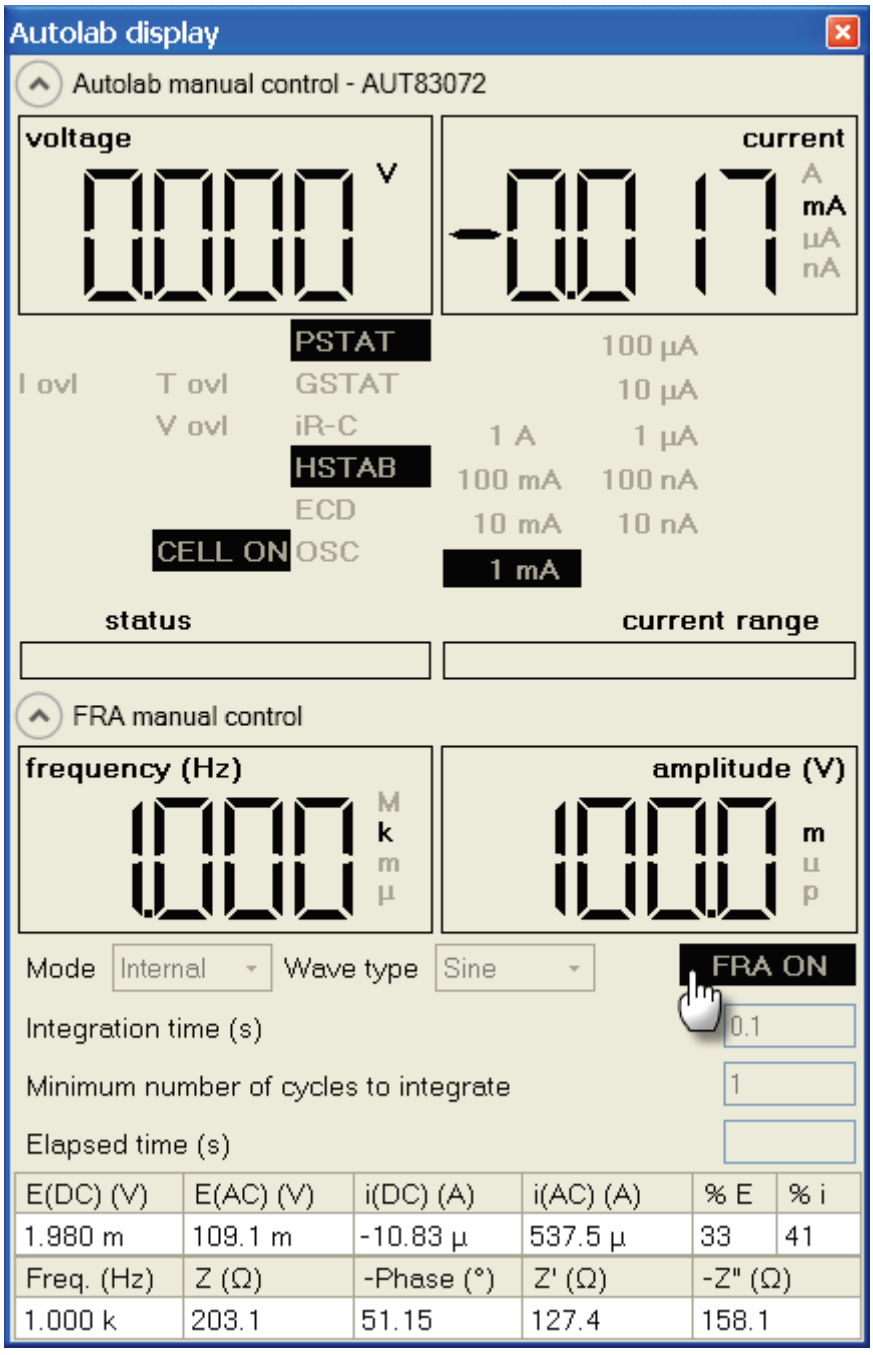


Figure 86 – The Autolab display with the FRA manual control

Pressing the **FRA ON** button switches on the FRA2 module and starts the manual measurement. The measured values are displayed at the bottom of the panel. It is possible to modify the amplitude or the frequency during the measurement.

Note: the measurements are repeated until the FRA ON button is clicked again to switch off the impedance analyzer.

More information on the use of the FRA manual control panel can be found in the **Impedance tutorial**, available from the Help menu.

Graphical user interface for Fit and Simulation

A graphical circuit editor has been added to the Fit and Simulation data analysis tool for impedance spectroscopy data. Using this tool, it is possible to create an equivalent circuit graphically, using the individual circuit elements and connections between these elements (see Figure 121).

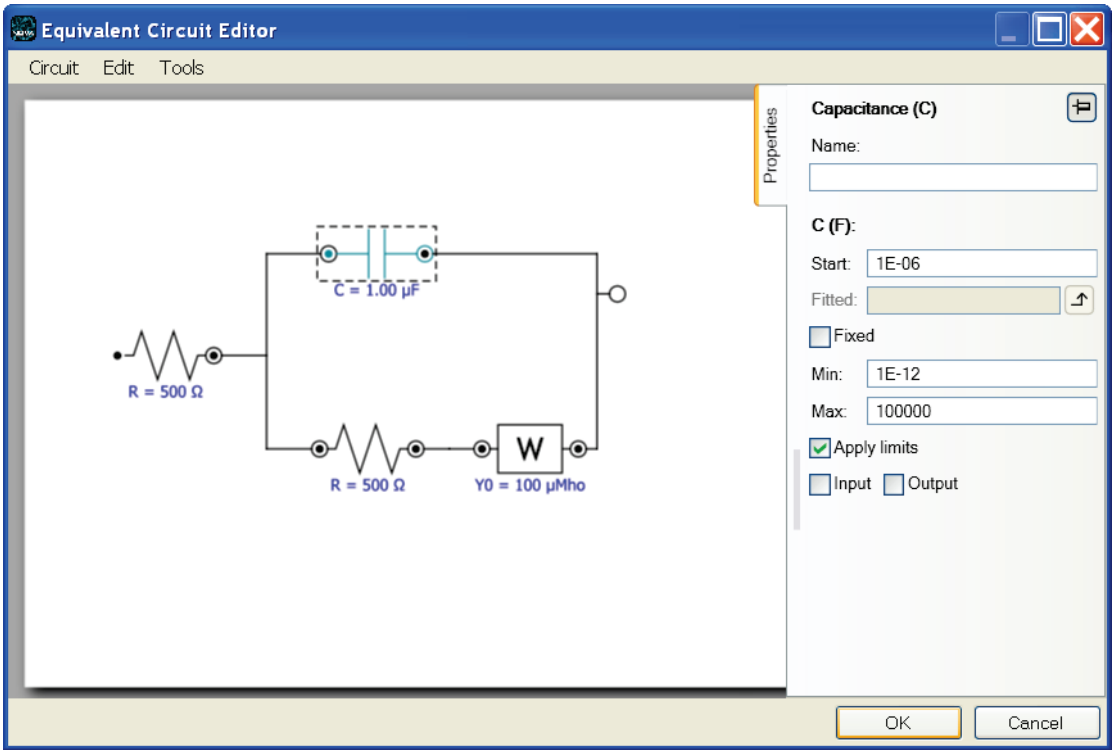


Figure 87 – A graphical circuit editor has been added to the Fit and Simulation analysis tool

Note: equivalent circuits can also be created using the traditional CDC syntax.

Fit results can be exported easily using the included reporting tool (see Figure 88).

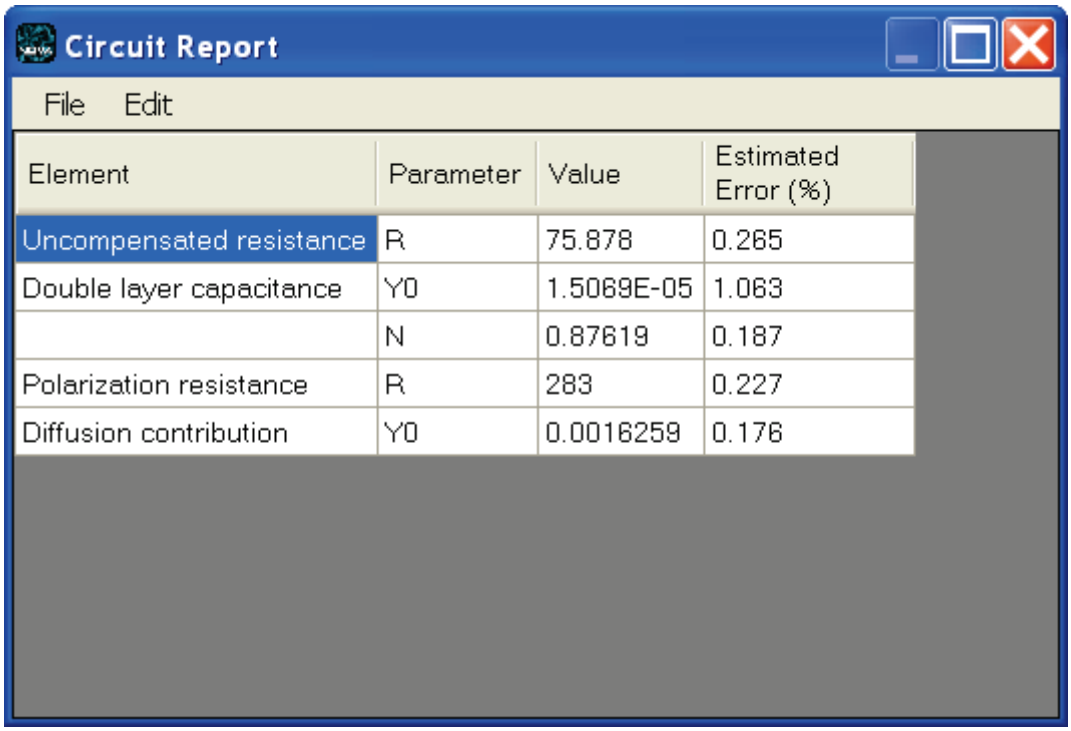


Figure 88 – The Circuit Report tool can be used to view the results

Moreover, an additional user-defined database, in which equivalent circuits can be stored for future use, has been created. This database can be defined through the database manager (see Figure 122).

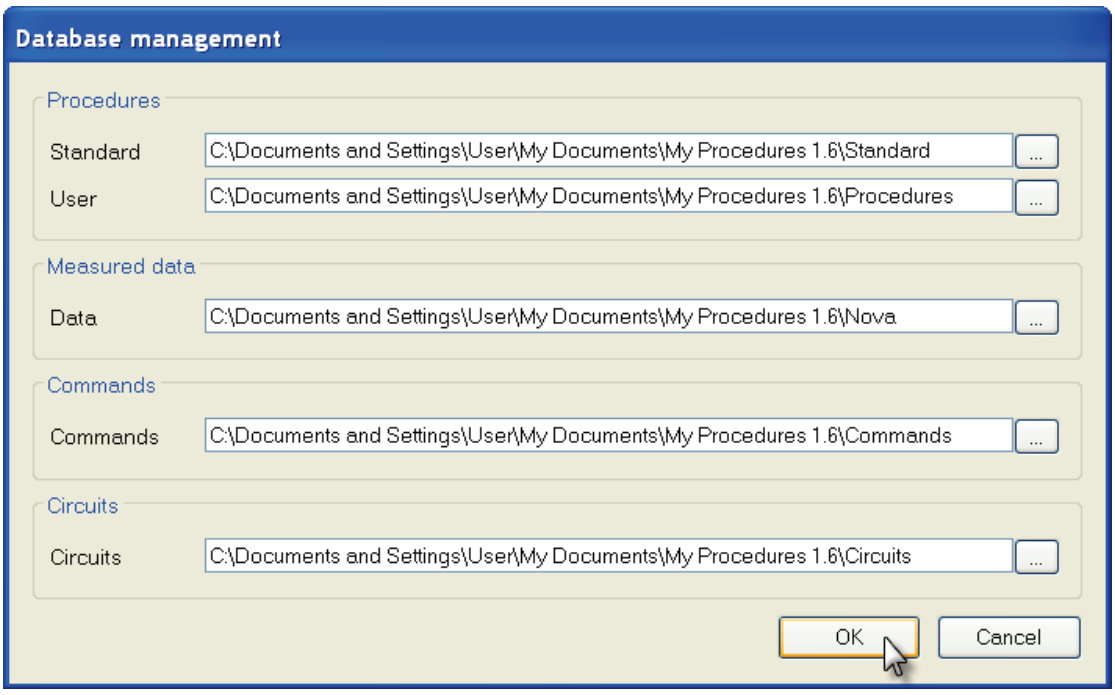


Figure 89 – The Circuits database has been added to the database manager

Note: more information about the new Fit and Simulation tool can be found in the Impedance spectroscopy tutorial.

Simplified commands and parameters

For more clarity, some advanced parameters have been hidden from view in the default procedure setup. These advanced parameters are still available and can be modified if required, but the modification of these parameters is only required for advanced measurements.

It is possible to switch from the default view to the advanced command view by using the toggle available in the View menu (see Figure 90).

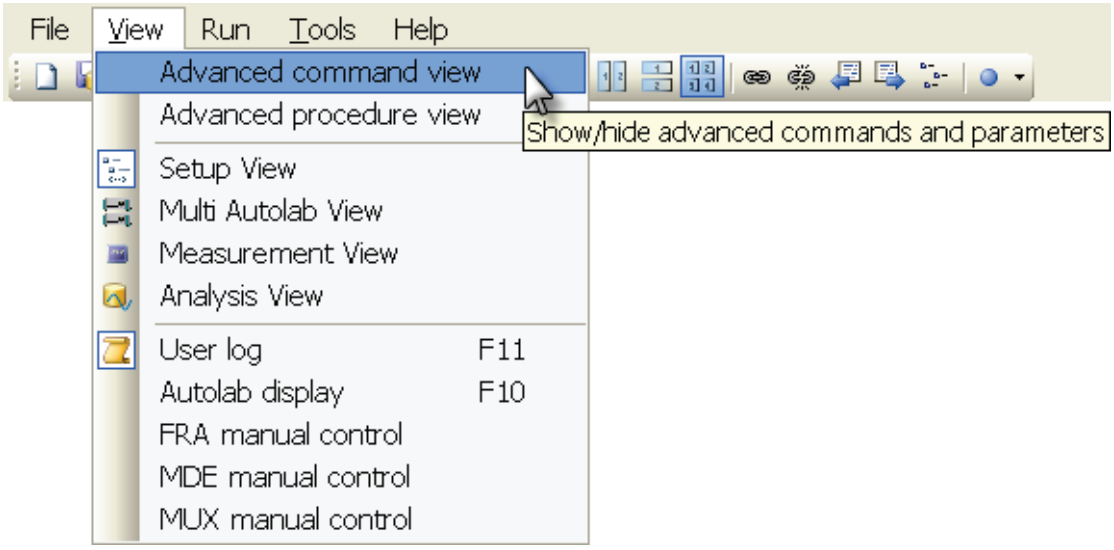


Figure 90 – The Repeat for each row command provides a table of one of more parameters

Switching to the Advanced command view displays the advanced commands in the commands browser and the advanced parameters in the procedure setup frame. Figure 91 shows a side by side comparison of the *FRA single frequency* command in normal mode and in advance command view.

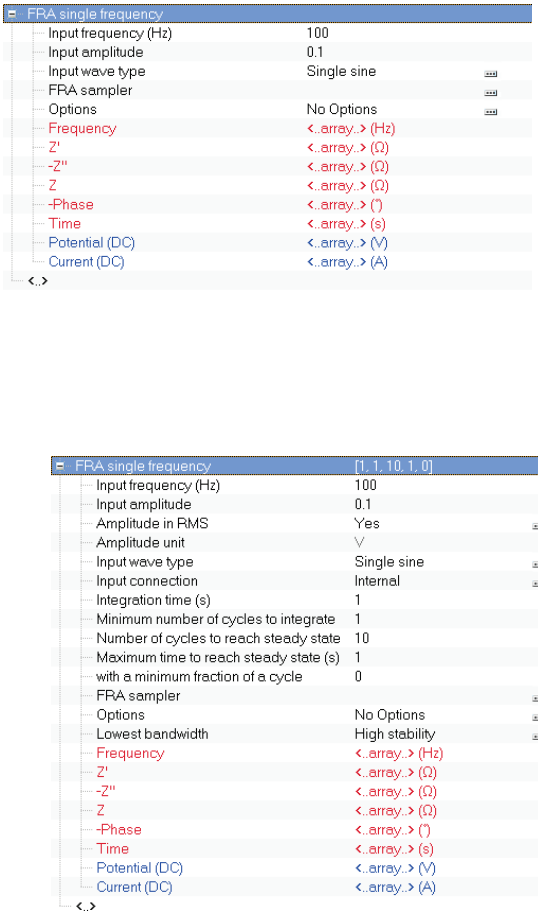


Figure 91 – Comparison of the FRA single frequency command, shown in default simplified mode (left) and in the advanced command view (right)

Support for MultiBA instruments

Version 1.6 of NOVA includes support for MultiBA devices. The MultiBA instrument is a special version of the modular Autolab PGSTAT (except the PGSTAT100) in which more than one BA module is installed. This provides the means to perform measurements on up to six working electrodes, sharing a common reference and counter electrode, at the same time.

Multiple BA modules, numbered #1 to #5, can now be selected in the Hardware setup (see Figure 92).

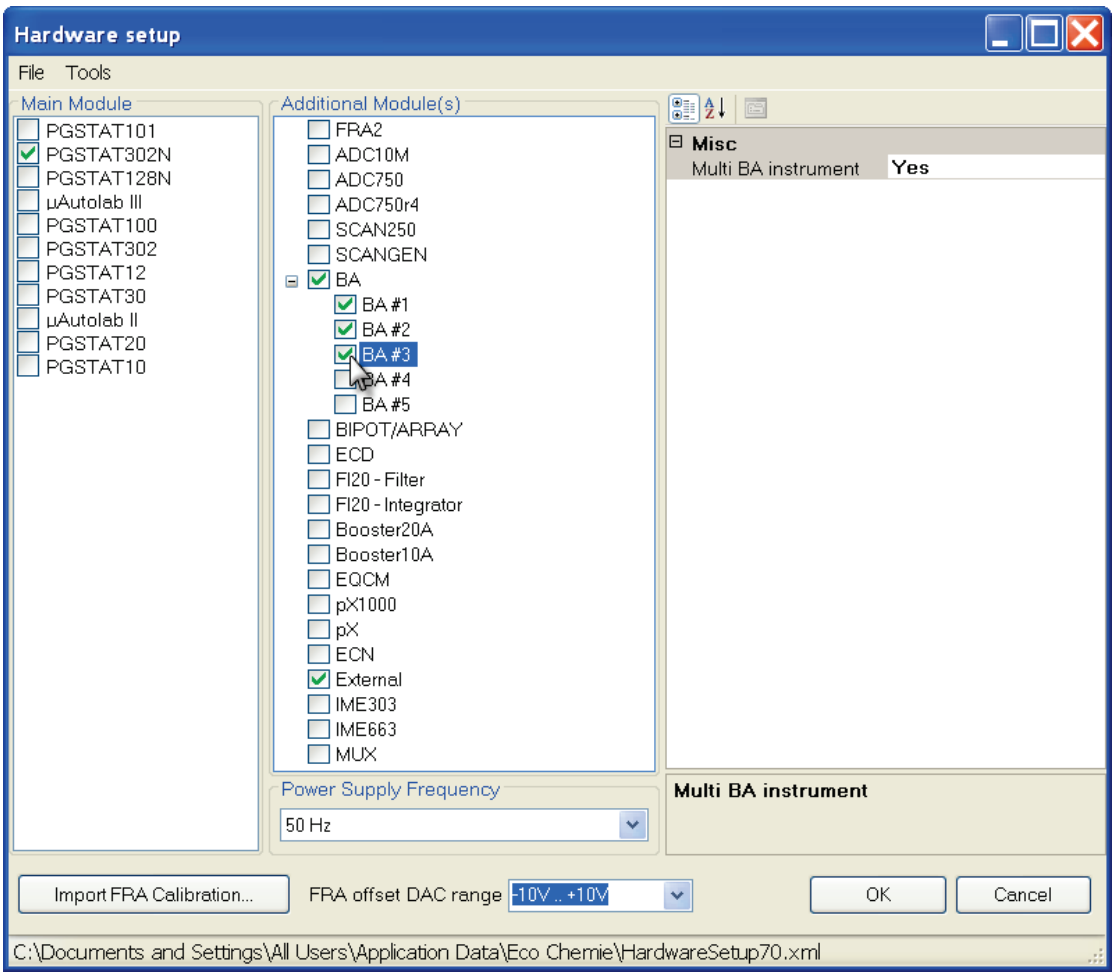


Figure 92 – Selecting multiple BA modules for a MultiBA instrument

The WE(x).Current and WE(x).Potential signals will be added to the Signal sampler. These signals can be sampled during electrochemical measurements (see Figure 93).

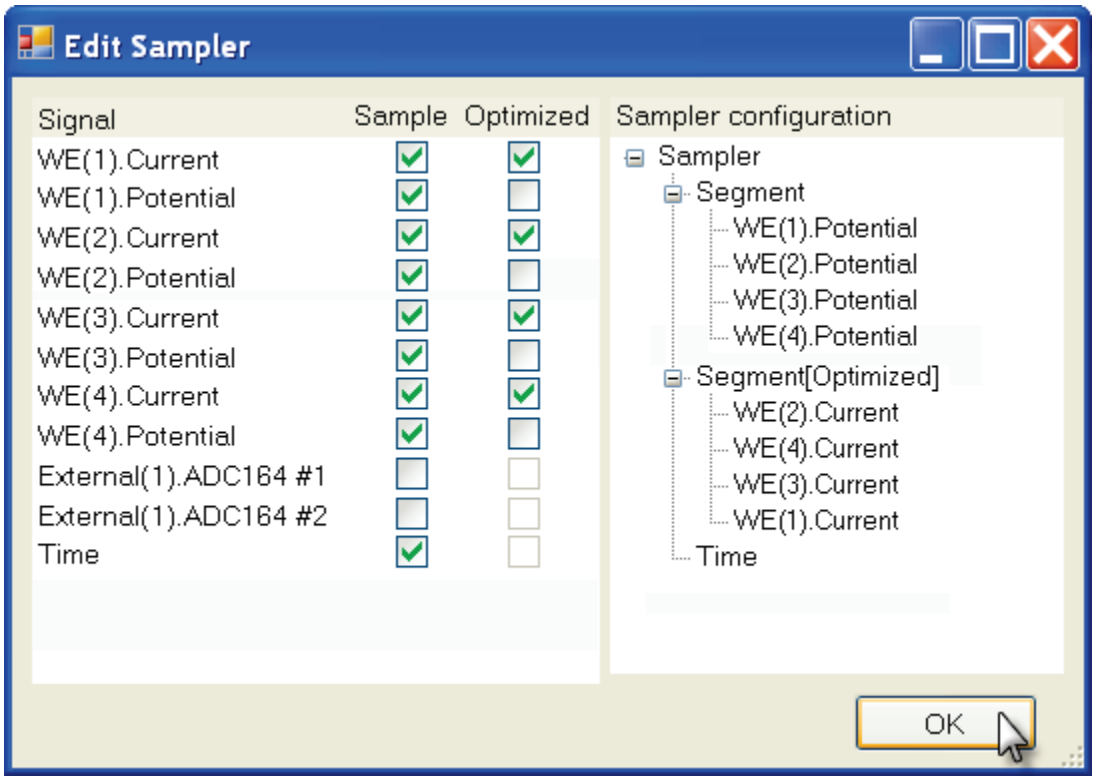


Figure 93 – The WE(x).Current and WE(x).Potential signals are available in the signal sampler

Note: only the signals of the selected modules are shown. In Figure 93, BA modules #2 and #3, corresponding to WE(3) and WE(4), respectively, are present in the instrument but not selected in the Hardware setup.

More information on the use of the MultiBA instruments in NOVA can be found in the **MultiBA tutorial**, available from the Help menu.

Multi Autolab support

Version 1.6 of NOVA includes support for multiple instruments. It is now possible to connect multiple Autolab instruments to the same computer and perform measurements using any of the connected devices. The maximum number of devices is limited to 8.

Selection of the active device is performed using a dedicated toolbar (see Figure 94). Available devices are identified by their serial numbers or by the serial number of the external USB interface, if applicable.

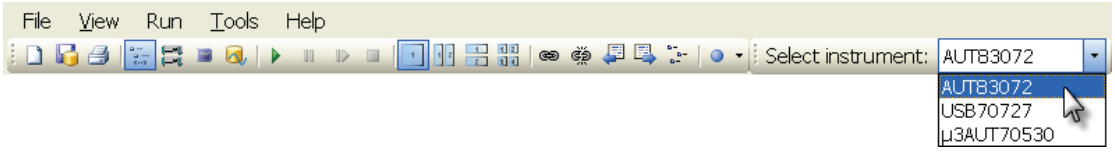


Figure 94 – A dedicated toolbar is can be used to select an instrument

Measurements can be performed on multiple instruments in the same way they are performed when a single instrument is connected to the computer. A single

procedure can run on any of the available devices. However, only one instrument can be used during the measurements in this mode.

It is also possible to control more than one device at the same time, in order to run the same or different procedures. This can be done by using the Multi Autolab view.

The Multi Autolab can be selected using the View menu or by clicking the button in the toolbar (see Figure 95).

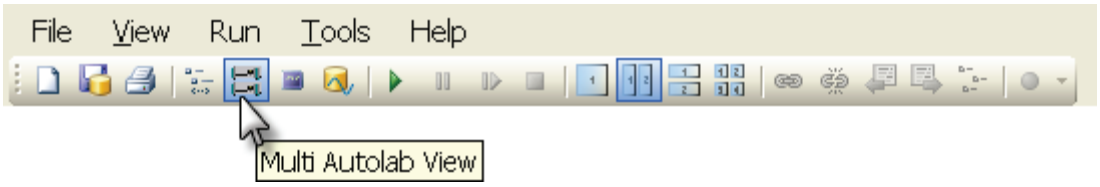


Figure 95 – The Multi Autolab view can be accessed using the View menu or the dedicated button in the toolbar

This view provides a dedicated interface through which two or more devices can be controlled (see Figure 96).

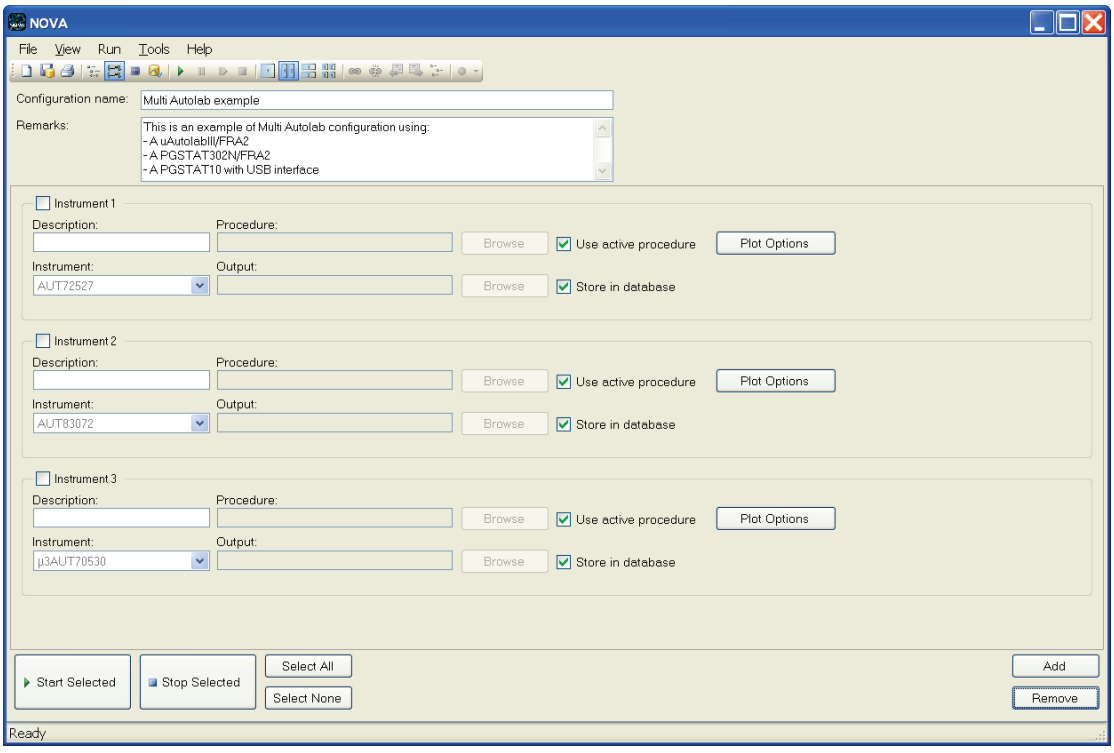


Figure 96 – The Multi Autolab view provides an interface through which two or more devices can be controlled at the same time

Note: more information on the control of multiple instruments can be found in the Multi Autolab tutorial, available from the Help menu.

Software synchronization command for Multi Autolab measurements

The *Multi Autolab software synchronization* command has been added to the Measurement – General group of commands. This command can be used create a synchronization point for two or more instruments in a procedure.

When two or more instruments perform this procedure in Multi Autolab mode, the synchronization commands will force the instruments to hold until the number of instruments holding at the synchronization point matches the value defined by the user in the procedure, or until the command reaches the time limit, if applied (see Figure 97).

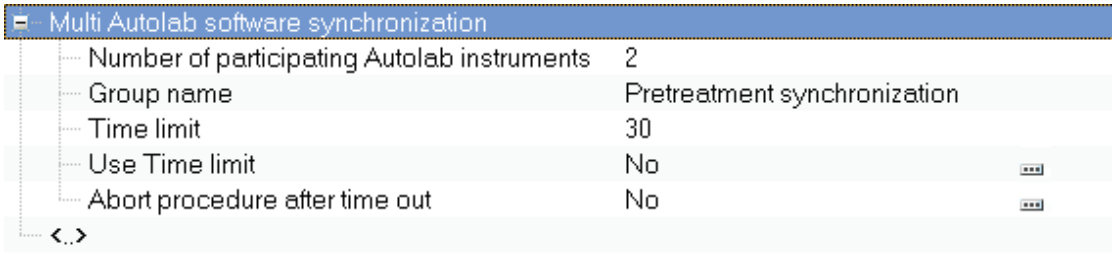


Figure 97 – The Multi Autolab software synchronization command can be used to synchronize two or more Autolabs during a Multi Autolab measurement

Note: the timing accuracy of the software synchronization command is 100 ms.

More information can be found in the Multi Autolab tutorial, available from the Help menu.

Instrument serial number and description in the database

To simplify data management in the database, each experiment is now logged with the identifying serial number and the configuration name, if specified, in the database frame (see Figure 98). This additional information can be used to find data sets more easily. It is possible to use the database for sorting the experiments using any of the available columns and to filter the database contents using the provided tools in order to display only specific measurements.

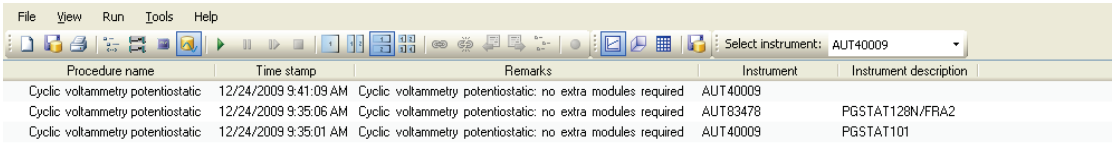

File View Run Tools Help
Select instrument: AUT40009
Procedure name | Time stamp | Remarks | Instrument | Instrument description
Cyclic voltammetry potentiostatic | 12/24/2009 9:41:09 AM | Cyclic voltammetry potentiostatic: no extra modules required | AUT40009
Cyclic voltammetry potentiostatic | 12/24/2009 9:35:06 AM | Cyclic voltammetry potentiostatic: no extra modules required | AUT83478 | PGSTAT128N/FRA2
Cyclic voltammetry potentiostatic | 12/24/2009 9:35:01 AM | Cyclic voltammetry potentiostatic: no extra modules required | AUT40009 | PGSTAT101

Figure 98 – The database frame includes an Instrument serial number column and an Instrument description column

Please refer to the User Manual and the Multi Autolab tutorial for more information.

Multi Autolab support in Diagnostics application

The diagnostics tool has been modified in NOVA 1.6. This application now supports multiple Autolab instruments. When the application starts it detects all available instruments connected to the computer (see Figure 99).

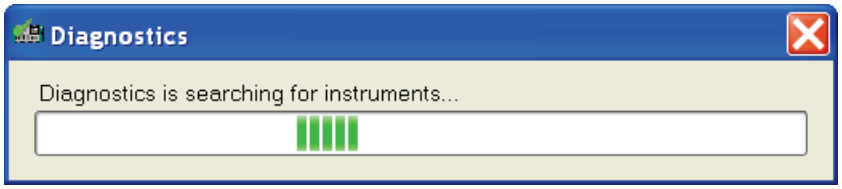


Figure 99 – The Diagnostics application automatically scans for all the connected instruments

Note: the test can only be performed on a single instrument at a time.

If more than one instrument is detected, a selection menu is displayed before the Diagnostics starts (see Figure 100).

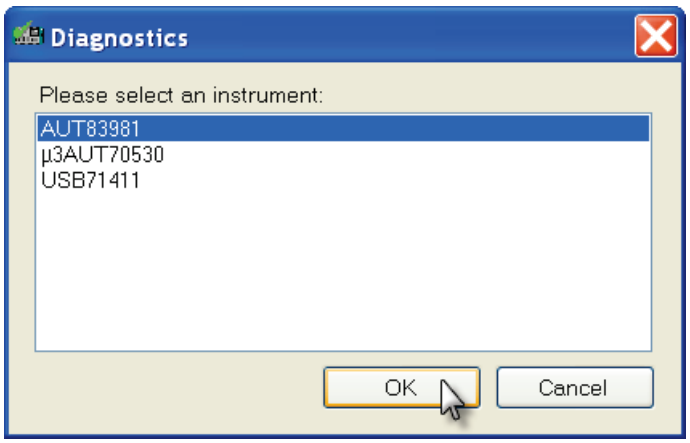


Figure 100 – A selection menu is displayed if more than one instrument is detected

Note: instruments with serial number beginning with AUT9 or with µ2AUT7, connected through an external USB interface, are identified by the serial number of the interface, USB7XXXX. Instruments with an internal USB interface, or instruments with serial number beginning with AUT7 connected through an external USB interface, are identified by their own serial number.

If the hardware setup of the connected instrument can be located on the computer, the diagnostics test can be performed immediately. Otherwise, the hardware setup for the connected instrument can be defined. Select the Hardware setup option from the Select menu (see Figure 101).

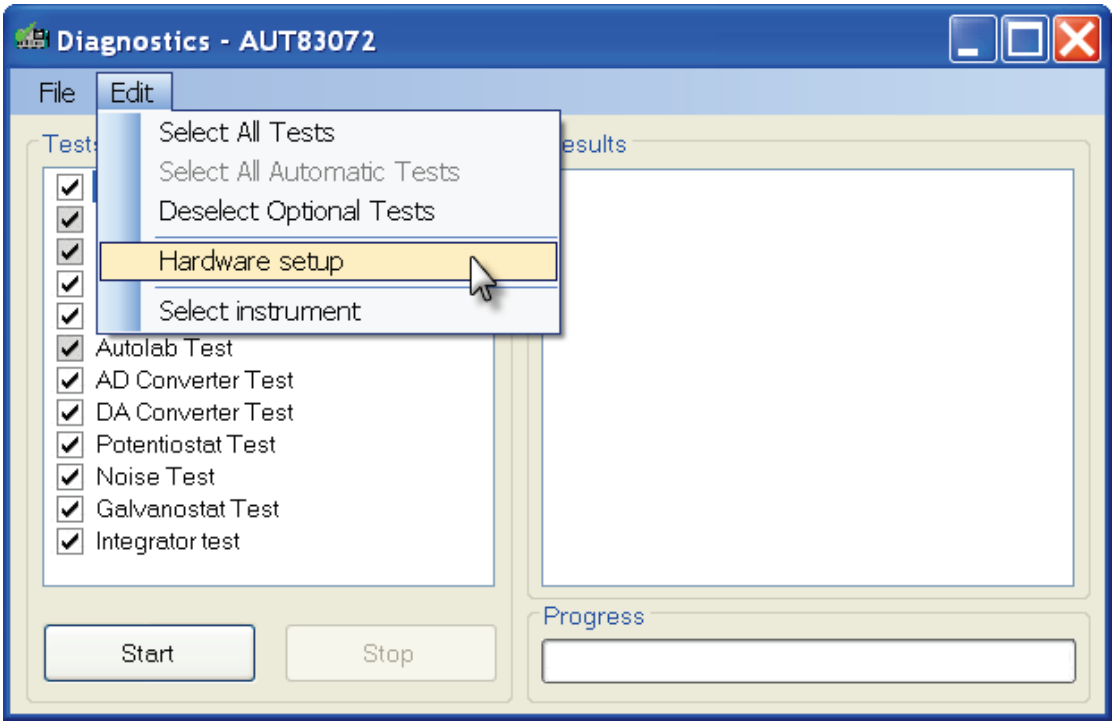


Figure 101 – Adjusting the hardware setup for the connected instrument

Procedure validation screen

The procedure validation screen has been redesigned in order to present errors and/or warning in a clear way. If errors or warnings situations are detected during the validation step, a window showing these errors and/or warnings will be displayed (see Figure 102).

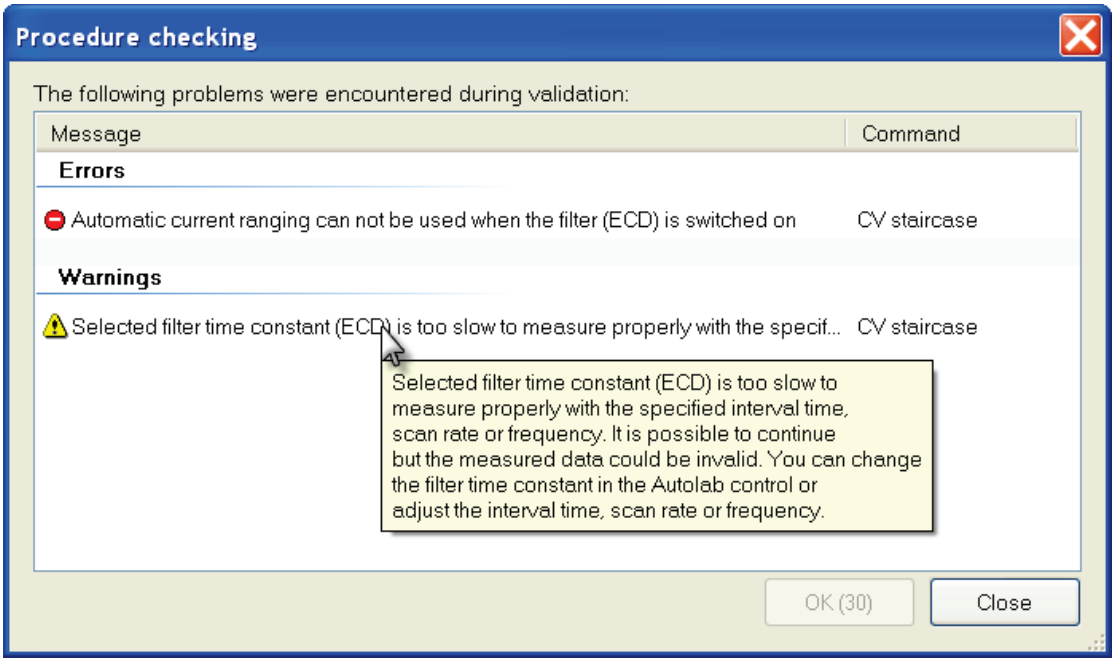

Procedure checking
The following problems were encountered during validation:
Message
Command
Errors
Automatic current ranging can not be used when the filter (ECD) is switched on
CV staircase
Warnings
Selected filter time constant (ECD) is too slow to measure properly with the specif...
CV staircase
Selected filter time constant (ECD) is too slow to measure properly with the specified interval time, scan rate or frequency. It is possible to continue but the measured data could be invalid. You can change the filter time constant in the Autolab control or adjust the interval time, scan rate or frequency.
OK (30)
Close

Figure 102 – The redesigned procedure validation screen now groups errors and warnings messages

If only warnings are detected, the procedure can be started by pressing the OK button, although it is recommended to verify the warning messages before starting the measurement.

FFT Analysis and FFT Smoothing

Two FFT related analysis tools (with matching commands in the Analysis – general group of commands have been added):

- **FFT Smooth:** Applies a smoothing on the measured data to filter out noise and spikes. The frequency domain data is first calculated through an FFT. One of four type of filtering strategies can be applied (low pass, high pass, band pass and band stop). The filtered data is reconverted to time domain after the filtering is applied.
- **FFT Analysis:** Calculates the frequency domain data from source time domain data through a FFT.

Both tools can be selected from the right-click menu (see Figure 103) or can be added as commands in a Nova procedure.

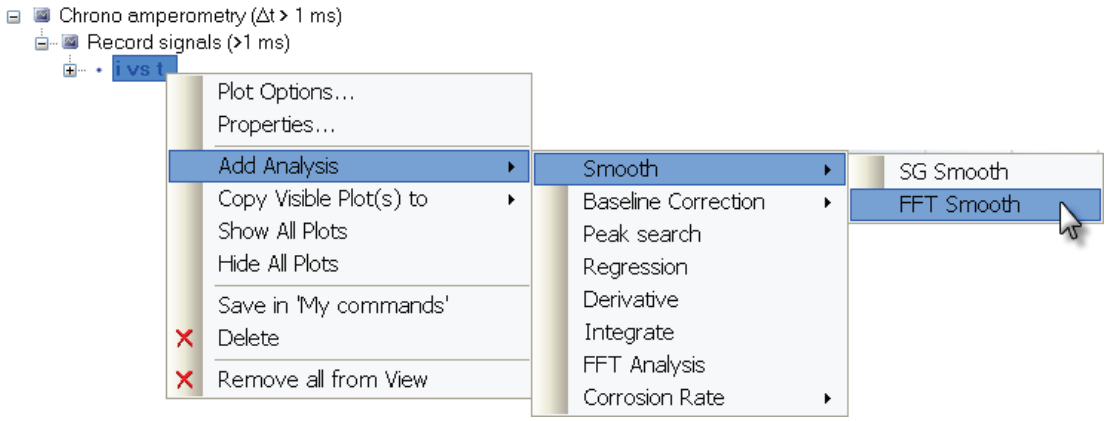


Figure 103 – Both the FFT Smooth and FFT Analysis tools have been added

More information on the use of these tools can be found in the User Manual, Chapter 4.

ECN Spectral noise analysis

A dedicated spectral noise analysis command has been added to Nova. This analysis tool can be used to analyze electrochemical noise data obtained using the ECN module or measured through the Autolab PGSTAT. This analysis tool is also available as a command in the Analysis – general group of command. This analysis tool can only be used in combination with data sets that include the Time, WE(1).Current and, WE(1).Potential or ECN(1).Potential (see Figure 104).

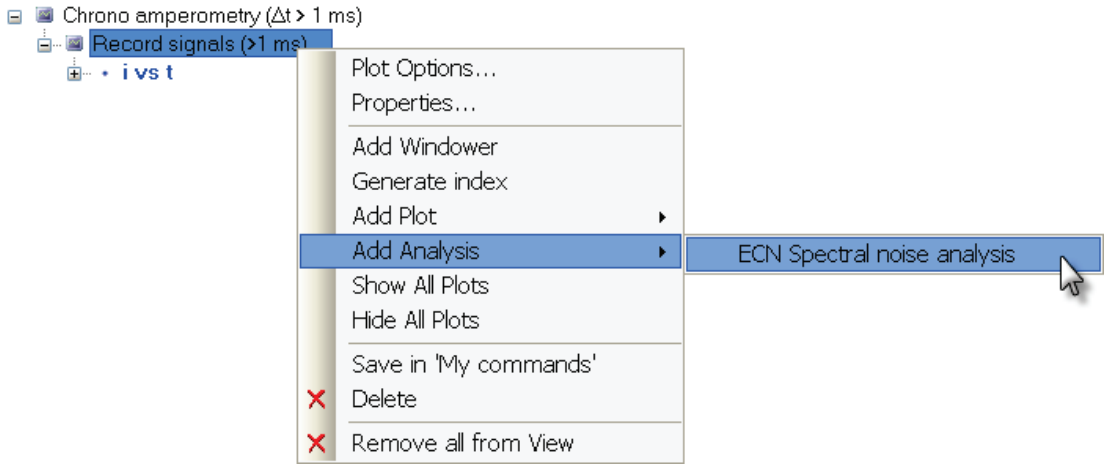


Figure 104 – The ECN Spectral noise analysis command has been added

Typical electrochemical noise analysis options are available in this analysis tool. It can be used to construct power spectrum density plots of potential, current and impedance for graphical analysis of noise data. Additional statistical indicators like noise resistance, pitting index, kurtosis and skewness are automatically calculated (see Figure 105).

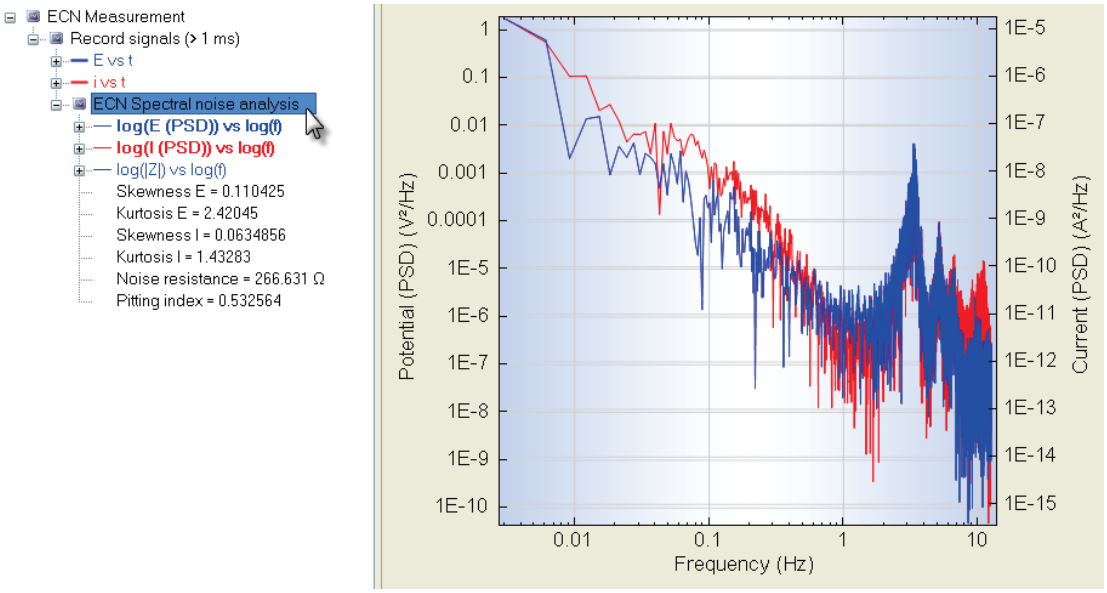


Figure 105 – An example of ECN spectral noise analysis data

Please refer to the ECN tutorial, available from the Help menu, for more information.

Clear plot button modification

The clear plot button, available in the Measurement view, has been modified in order to allow the user to clear all the plots at once (by clicking the clear plot button,) or to clear one of the specific plot by extending the context menu (by clicking the arrow button, ,located next to the clear button). Any one of the four plots can be cleared through this context menu (see Figure 161).

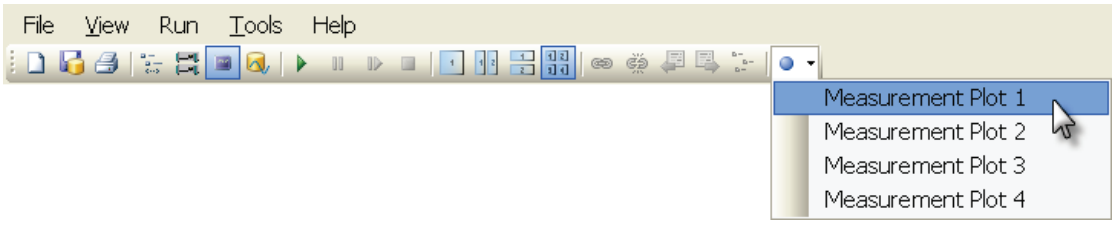


Figure 106 – It is possible to clear a specific plot in the measurement view by extending the Clear plot button

Dynamic command parameters

This version of NOVA clarifies the concept of *Dynamic command parameters*. Contrary to normal command parameters, belonging to individual commands, like the Scan rate parameter for a Cyclic voltammetry command or the interval time in a Chrono methods command, dynamic command parameters are parameters that are generated by data handling or data analysis commands, during a measurement. Dynamic command parameters therefore have no initial values and they are generated during experiments.

For example, the slope calculated by a linear regression on measured data, can only be provided once the data is collected and the calculation performed. The same applies to the value of a Constant phase element impedance obtained by fitting experimental data.

NOVA now allows the user to use these dynamic command parameters in the same way as any other parameter. The results of calculations or data handling steps can be linked to other parameters or can be plotted during a measurement. For example, the result of a linear regression can be used in a procedure, plotting the intercept versus the square root of the scan rate.

To identify dynamic command parameters in the procedure editor, these parameters are now shown in **blue**. Other parameters are shown according the following color convention:

- **Red parameters**: measurable electrochemical signals (through the signal sampler or a dedicated sampler)
- **Black parameters:** command parameters that can be edited
- **Grey parameters:** command parameters that cannot be edited and are calculated based on the user-defined command parameter values.

Figure 107 shows an example of the four types of parameters in the procedure editor.

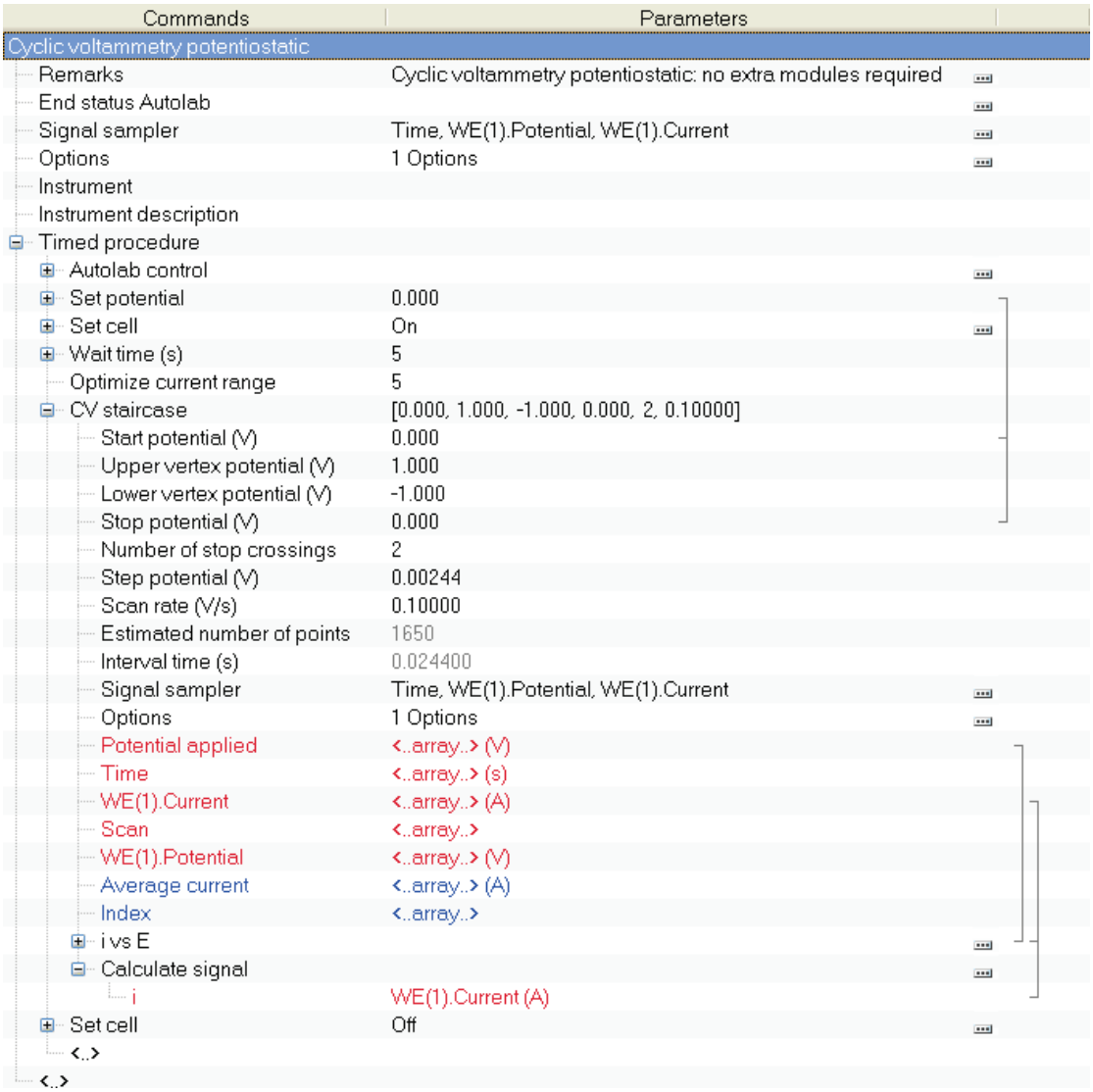


Figure 107 – An example showing the four types of parameters in the procedure setup

In this example, WE(1).Current is shown in red because it is a measured value, scan rate is shown in black since it is a command parameter, the interval time is shown in grey because it cannot be edited and it is calculated from the values of the scan rate and the step potential. The average current is a calculated value, generated by the *Calculate signal* command and it is therefore shown in blue. This parameter is a dynamic parameter since it is calculated during the experiment.

Dynamic command parameters are very useful for advanced procedure building. Figure 108 shows an example of the dynamic command parameters used in a procedure. Impedance measurements are repeated a number of times and fitted using a R(RQ) equivalent circuit. The fitted values of the circuit elements are dynamic command parameters and can be used to create plot #3 and plot #4, showing the fitted values versus the repeat number.

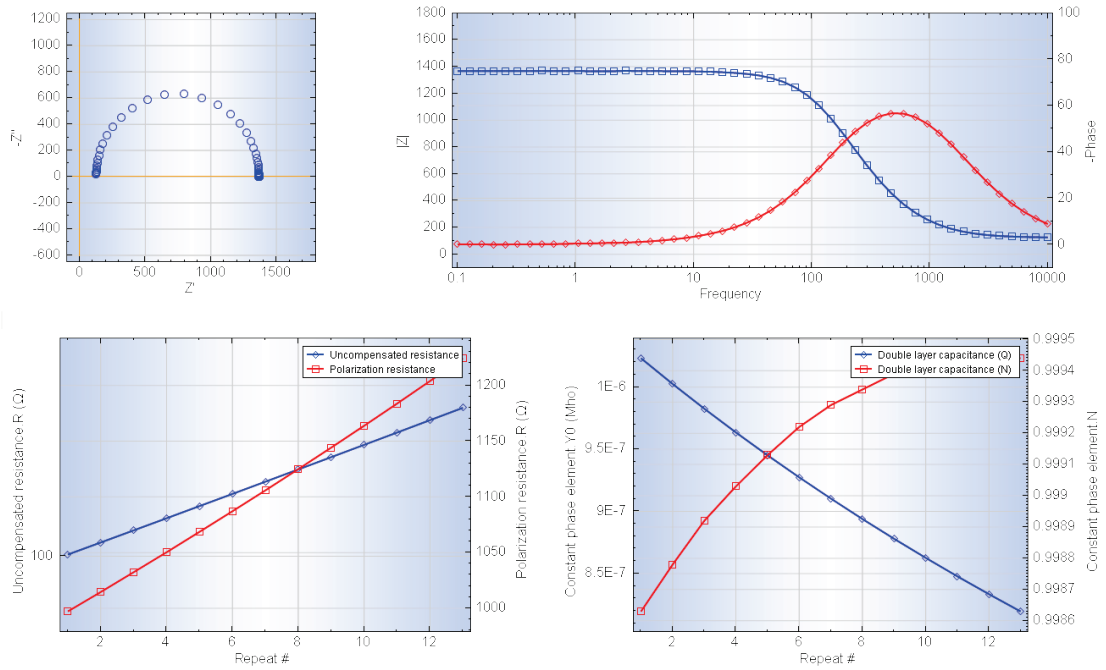


Figure 108 – Using Dynamic command parameters during a measurement: plot #1 and plot# 2 show raw impedance data, plot #3 and plot #4 show calculated values dynamically added by the *Fit and simulation* command

Repeat for multiple values

A new type of repeat loop, *Repeat for multiple values,* has been added to the Control group of commands. This command is similar to the *Repeat for each value* command. The difference with respect to the latter is that the *Repeat for multiple values* command can be used to define a Table of values, containing one or more columns (see Figure 109).

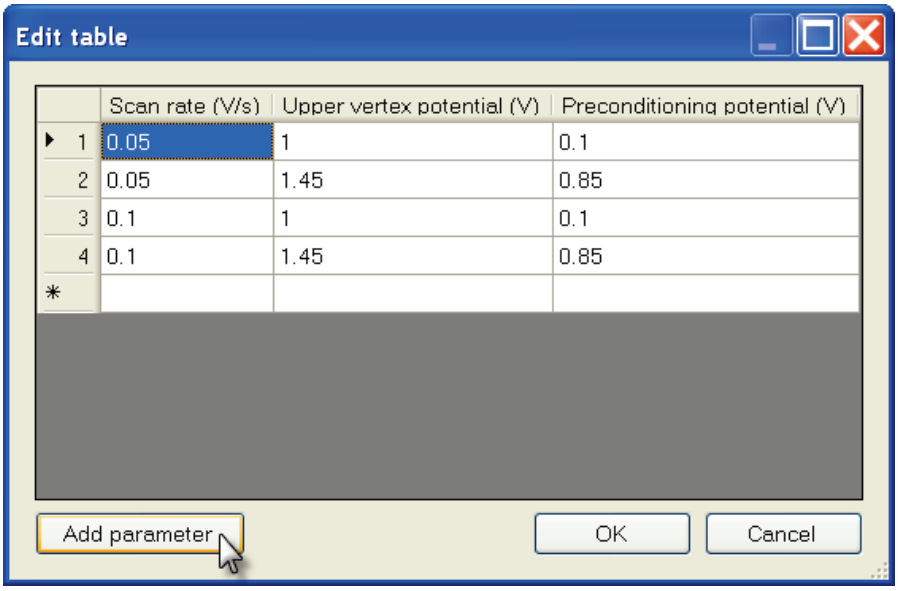


Figure 109 – The Repeat for multiple values command provides a table of one of more parameters

Note: the number of values in each column must be the same.

During the measurement, the commands in this new type of repetition loop will be repeated for each row of the table. A possible example is shown in Figure 110. In this example, the three parameters defined in the table shown in Figure 109 are linked to the Scan rate, Upper vertex potential and the Potential value defined in the Set potential command, respectively.

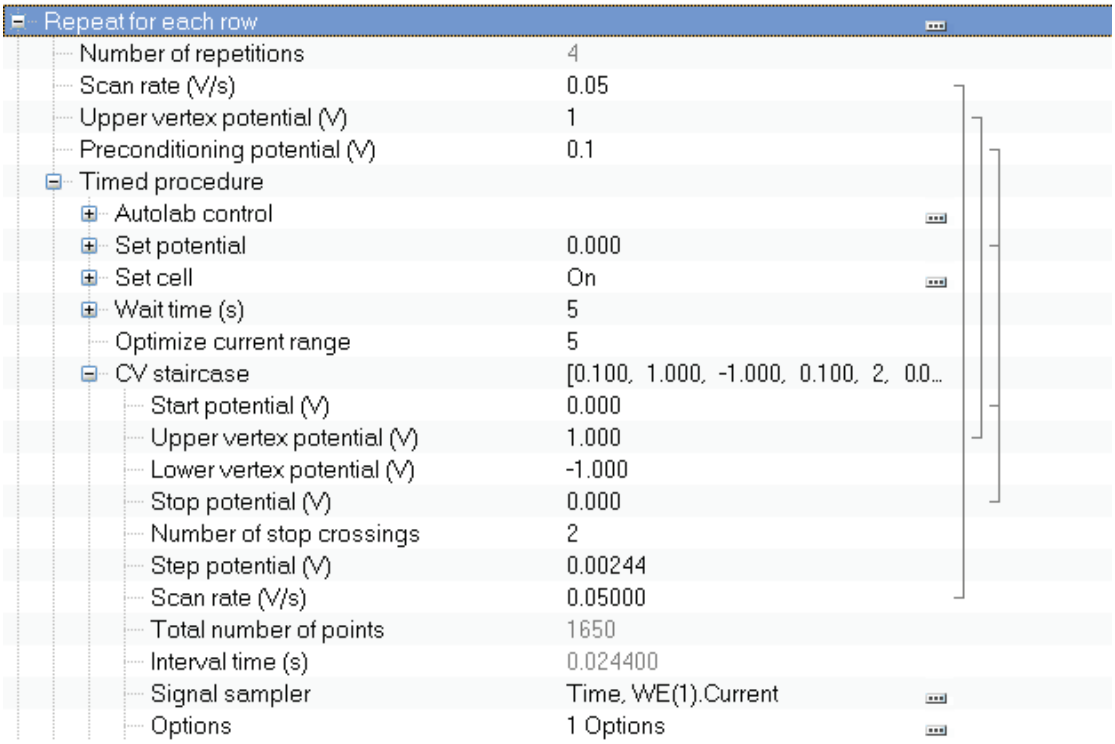

Repeat for each row
Number of repetitions 4
Scan rate (V/s) 0.05
Upper vertex potential (V) 1
Preconditioning potential (V) 0.1
Timed procedure
Autolab control
Set potential 0.000
Set cell On
Wait time (s) 5
Optimize current range 5
CV staircase [0.100, 1.000, -1.000, 0.100, 2, 0.0...
Start potential (V) 0.000
Upper vertex potential (V) 1.000
Lower vertex potential (V) -1.000
Stop potential (V) 0.000
Number of stop crossings 2
Step potential (V) 0.00244
Scan rate (V/s) 0.05000
Total number of points 1650
Interval time (s) 0.024400
Signal sampler Time, WE(1).Current
Options 1 Options

Figure 110 – A possible use of the Repeat for each row command

The measurement will therefore be repeated, using the values defined in each row for the three parameters.

Autolab display with collapsible panels

The Autolab display has been redesigned in this version of NOVA. It is now possible to add or remove panels to the Autolab display, by choosing the required options in the View menu (see Figure 111).

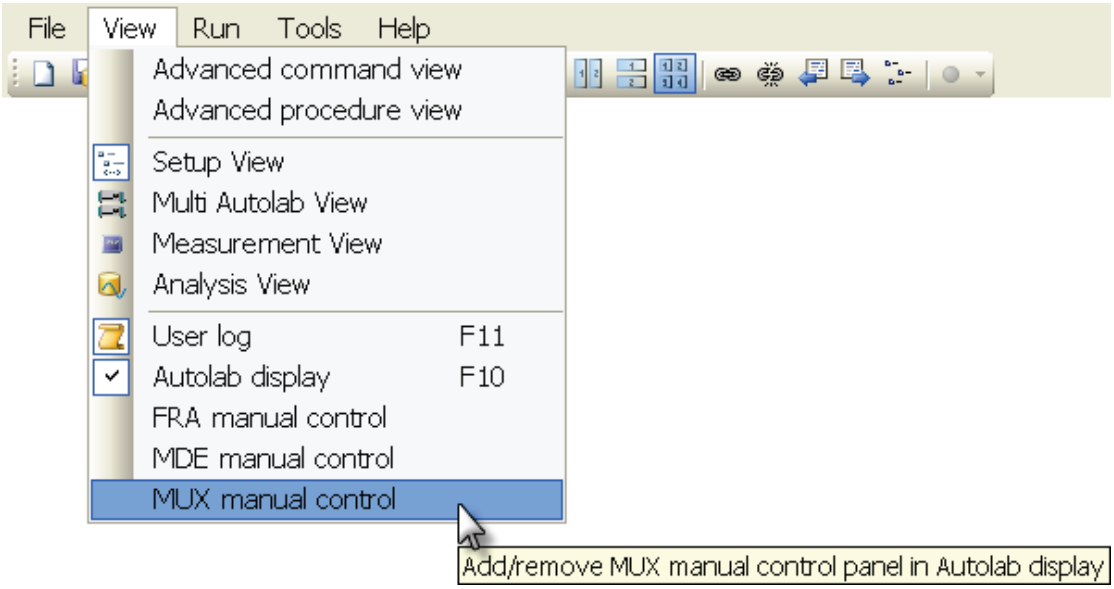


Figure 111 – Adding the MUX manual control panel to the Autolab display

Another example is shown in Figure 85 and Figure 86 (see section 0).

Each panel provides additional manual control over the instruments or the accessories connected to the instrument (see Figure 112).

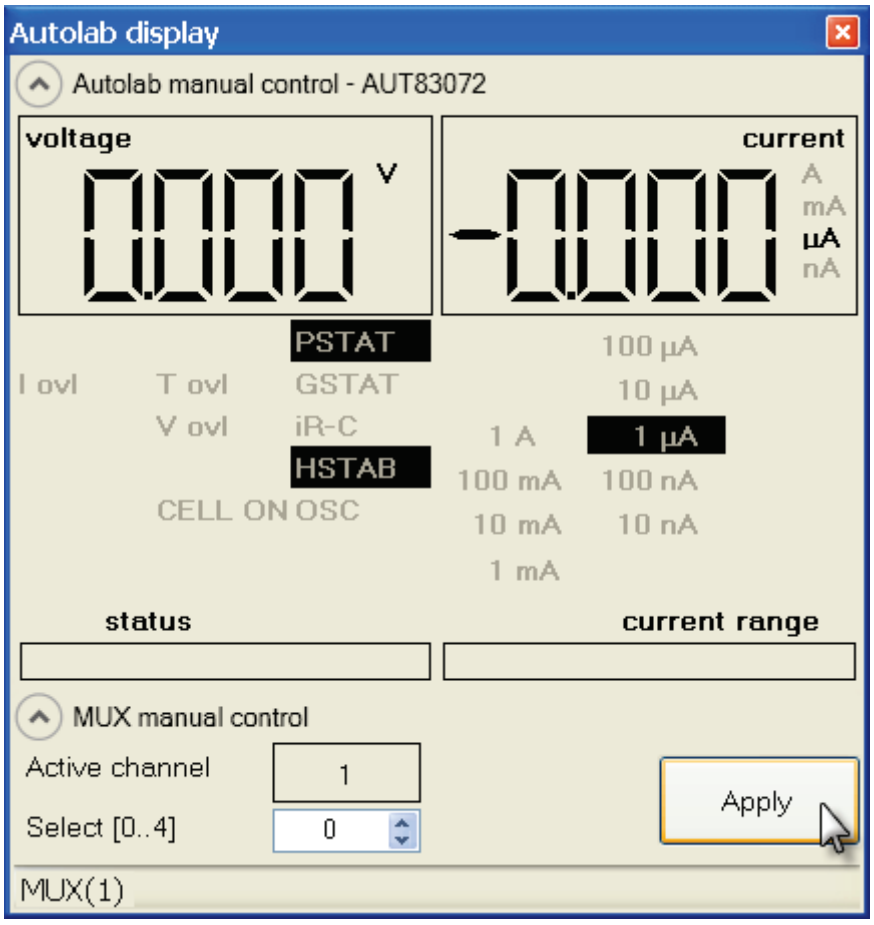


Figure 112 – The MUX manual control panel provides a direct interface to the MUX module

At any time, the panels can be collapsed and expanded by clicking the button in the top left corner of each panel (see Figure 113).

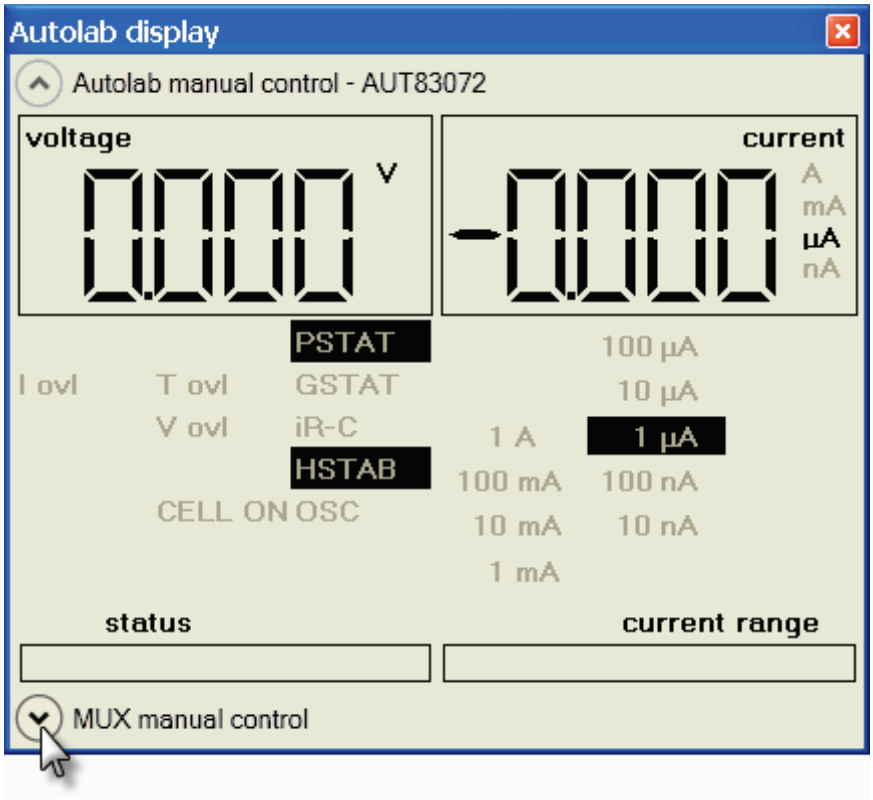


Figure 113 – Collapsing the MUX manual control panel

Pressing the button expands the panel again.

Current interrupt and positive feedback procedures

Two current interrupt procedures (i-Interrupt and i-Interrupt high speed) are now provided in the Autolab group of procedures. These procedures can be used to determine the uncompensated resistance of the cell, using the current interruption method. The i-Interrupt high speed procedure uses the fast sampling ADC module (ADC10M or ADC750).

These procedures can be used with all the instruments fitted with the iR compensation circuit[5]. Figure 114 shows an example of current interrupt measurement recorded using the provided procedure on the Autolab dummy cell.

[5] This option is not available with the PGSTAT10 and the µAutolab II/III.

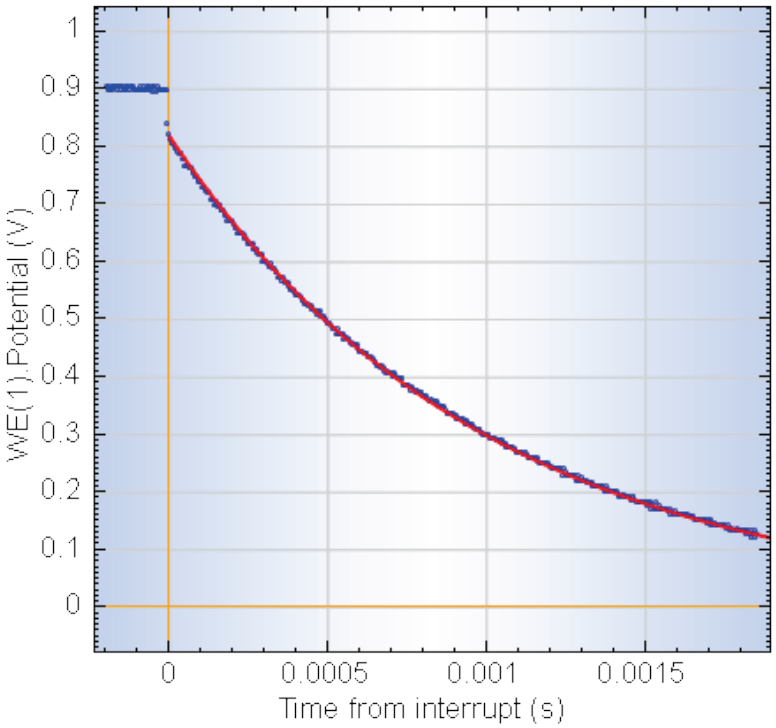


Figure 114 – Example of data obtained with the i-Interrupt high speed procedure

The recorded potential transient is automatically fitted and the calculated value of the uncompensated resistance is displayed in the Autolab display window (Figure 115). The transient is fitted using an exponential regression and a linear regression, yielding values of Ru exponential and Ru linear, respectively.

Note: the commands used in the i-Interrupt and the i-Interrupt high speed procedures are available in the Measurement – general group.

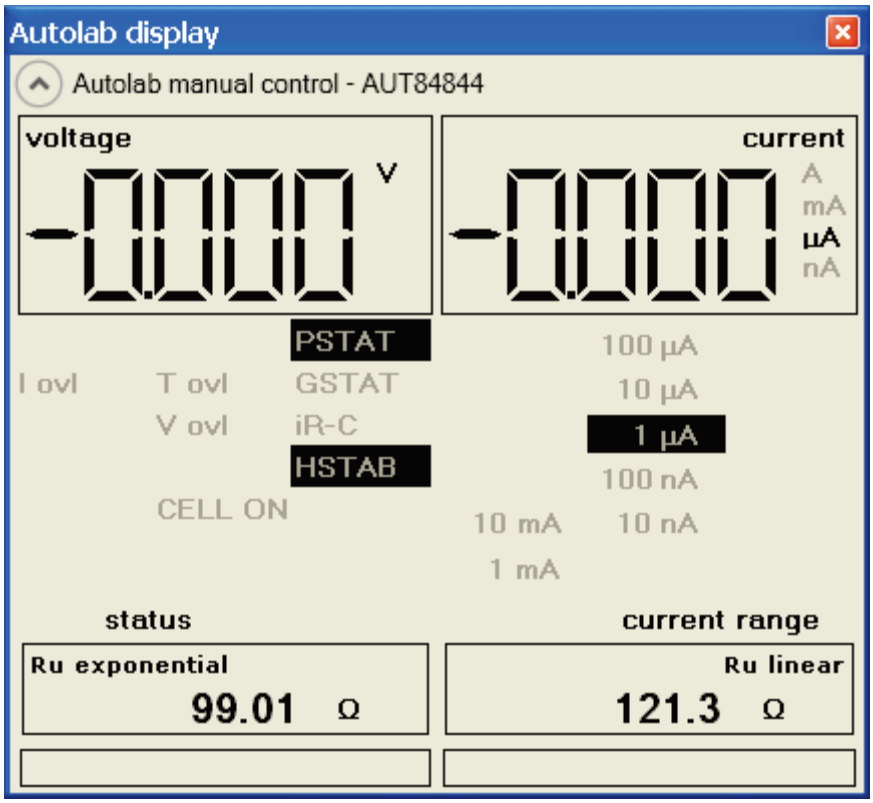


Figure 115 – The results of the fitting of the transient are shown in the Autolab display

Additionally, a Positive feedback procedure is supplied in the Autolab group of procedures. With this procedure, it is possible to fine tune the value of the uncompensated resistance estimated from the current interrupt procedures.

Figure 116 shows an example of four positive feedback measurements performed on the Autolab dummy cell, using compensated resistance values of 0, 95, 98 and 102 Ohm, respectively. The correct value of the uncompensated resistance can be determined by trial and error by detecting the point at which the response of the cell becomes a ringing oscillation.

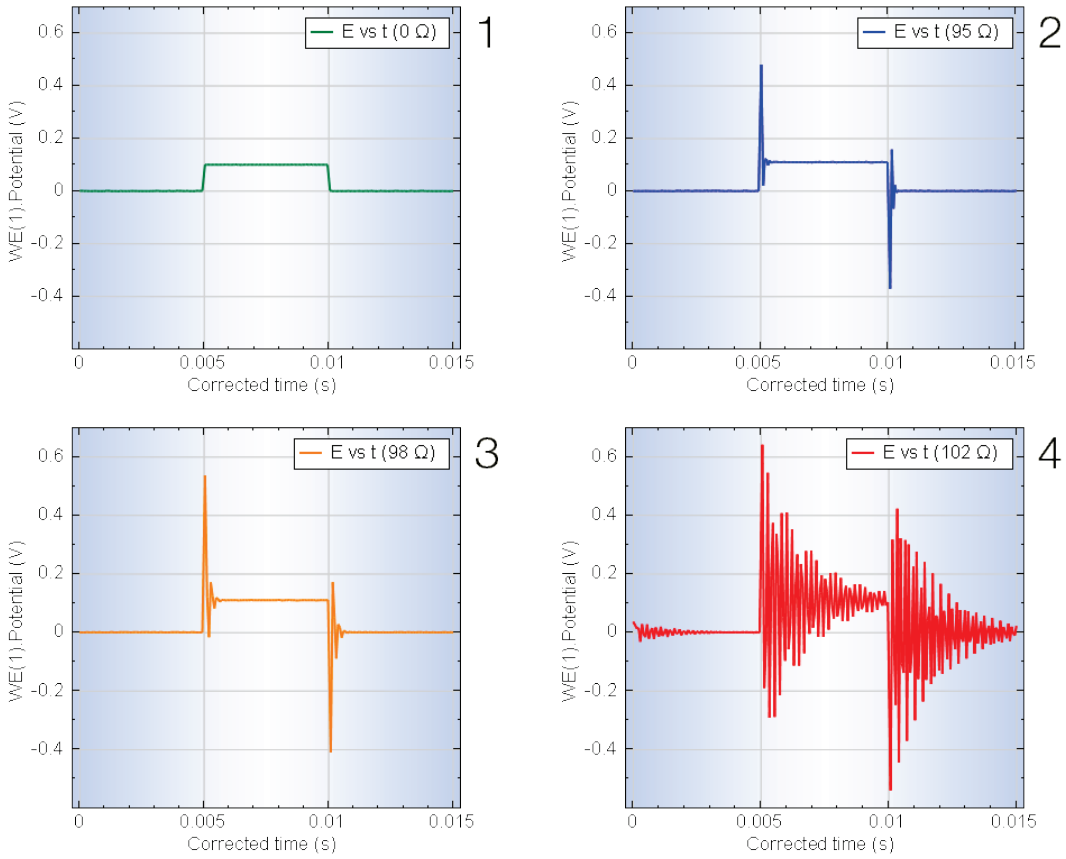


Figure 116 – Four different positive feedback experiment (plot 1 – green line: 0 Ohm, plot 2 – blue line: 95 Ohm, plot 3 – orange line: 98 Ohm, plot 4 – red line: 102 Ohm)

More information on the use of the i-Interrupt and Positive feedback procedures can be found in the iR Compensation tutorial, available from the Help menu.

External .NET applications support

External applications can be used from NOVA using dedicated commands. This option is for advanced applications only and requires the user to be familiar with software programming. A tutorial and some examples are provided in the installation folder[6].

Avantes spectrometer support

Basic support for Avantes spectrometers is available. Presently, support of these devices is possible through the External .NET commands. For more information, contact Metrohm Autolab B.V. (nova@metrohm-autolab.com).

[6] This information can be found in the Shared DataBases\Tutorials\External DOTNET DLL folder located in the installation folder.

NOVA 1.5 Release notes (Released 01/06/2009)

Introduction

These notes provide an overview of the new features introduced in NOVA 1.5 compared to the previous release.

The following items have been added to NOVA 1.5:

- A new set of tutorials, available from the Help menu

- Support for the modules

  - pX
  - ECN
  - FI20 – Filter
  - MUX
  - IME663 & IME303
  - Booster10A for the PGSTAT128N
  - ADC750 revision 4.0
  - PGSTAT101

- Improvements and additions

  - Voltammetric analysis techniques
  - Manual control of the Hg drop electrode (IME663 or IME303)
  - Manual control of the MUX
  - New user interface for Autolab control command
  - Manual control of the instrument through Autolab display
  - Skip button
  - Reverse button
  - Multiple plots in measurement view and overlays
  - Send email command
  - Check online for updates
  - New data handling commands
  - Timed procedure inside a FRA frequency scan
  - New FRA commands
  - Post measurement check
  - Save data option
  - Hardware summary in the About menu
  - Improved support for Metrohm devices
  - Autolab control in options
  - Wait on DIO trigger
  - New Autolab procedures
  - Test of Autolab modules

Previous NOVA versions and NOVA 1.5

It is possible to install more than one version of the NOVA software on the same computer. Installing version 1.5 does not upgrade previously installed versions. However, it is not possible to use both software packages at the same time and data sets obtained with NOVA 1.5 cannot be used with previous versions of NOVA. The opposite situation is possible, using the conversion tools that are installed together with version 1.5.

Tutorials

New tutorials have been added to this version of NOVA. The tutorials are available from the Help menu (see Figure 117).

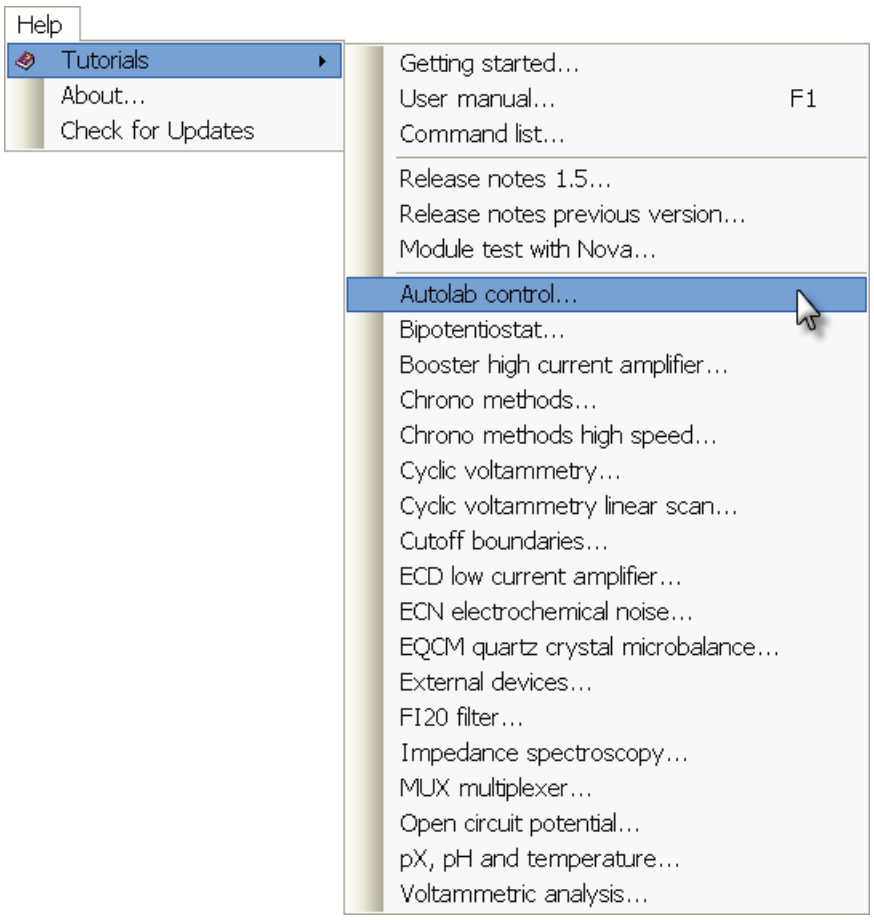


Figure 117 – New tutorials are available from the Help menu

Modules support

NOVA 1.5 introduces the support for the pX, ECN, MUX, FI20 – Filter modules and the for the IME663 and IME303 interfaces to the Hg drop electrode stands. Support for the Booster10A in combination with the PGSTAT128N is also provided.

Hardware support

The hardware setup of NOVA 1.5 now includes support for the ADC750 rev. 4, ECN, pX, FI20 – filter and MUX modules. The PGSTAT101 is also supported. The external signals can now be conveniently edited using a dedicated menu (see Figure 160). A special conversion function is provided for eSPR signals.

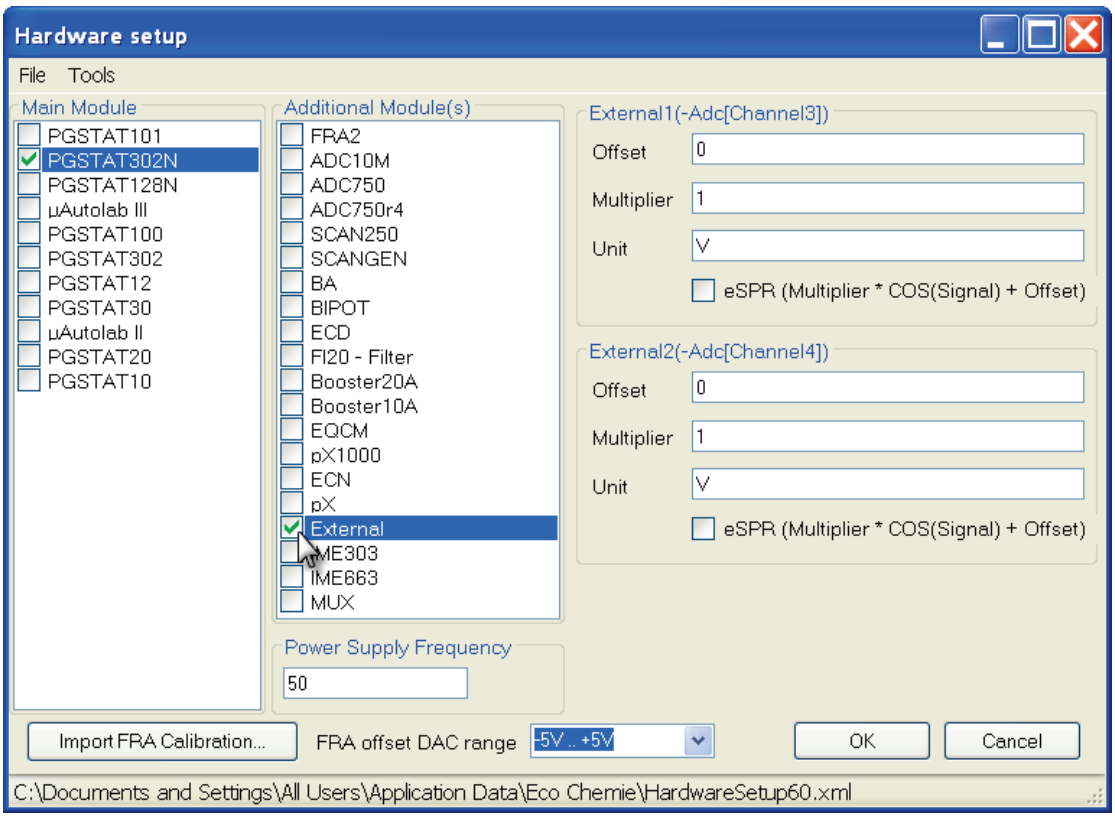


Figure 118 – The hardware setup window

Voltammetric analysis techniques

This new version of NOVA introduces the most commonly used voltammetric analysis (VA) techniques. These techniques can be used on solid electrodes or on a mercury drop electrode. The following techniques are now supported:

- Sampled DC
- Normal pulse
- Differential pulse
- Differential normal pulse
- Square wave

The commands required for these measurements can be found in the Measurement – voltammetric analysis group of commands (see Figure 119). The Timed procedure for voltammetric analysis provides a generic template for VA measurements.

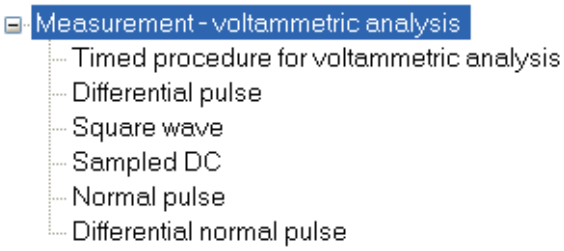


Figure 119 – The Voltammetric analysis commands

Note: it is possible to use these commands in polarographic mode (refer to the user manual for more information).

Alongside the VA measurement commands, additional commands to control the mercury drop electrode have been added to the Measurement – general group (see Figure 120):

- **Purge**: this command defines the duration of the purge step (the stirrer is always switched on when the N_2 purging is on).
- **Set stirrer**: this command controls the stirrer of the VA stand.
- **Create new drop**: this command creates n new drop by activating the drop knocker on the VA stand.

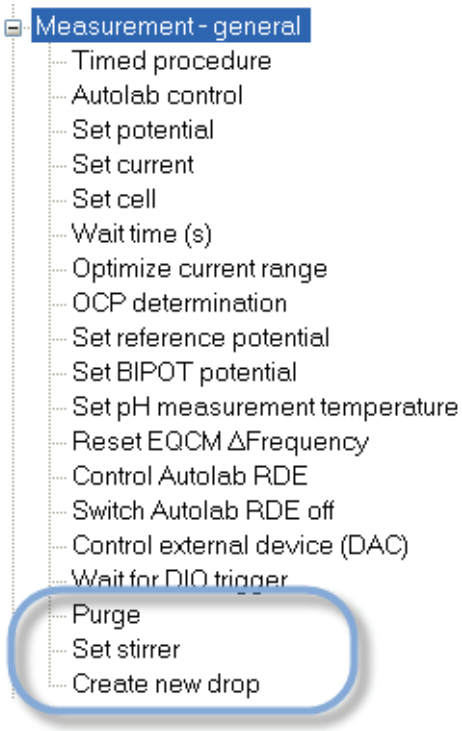


Figure 120 – Three additional command related to the control of the mercury drop electrode have been added to the Measurement – general group

Manual control for Mercury Drop Electrode (MDE)

Manual control over the Mercury Drop Electrode (MDE) is provided in the View menu (see Figure 121). This can be used to manually control the Metrohm VA 663 Stand or the PAR 303/303A Stand through the IME663 and the IME303, respectively.

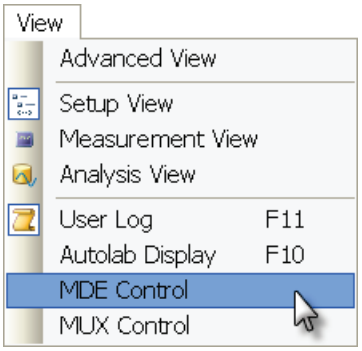


Figure 121 – Manual control of the MDE is provided in the View menu

Through the MDE control it is possible to manually switch purging and stirring on and off and create new drops (see Figure 122).

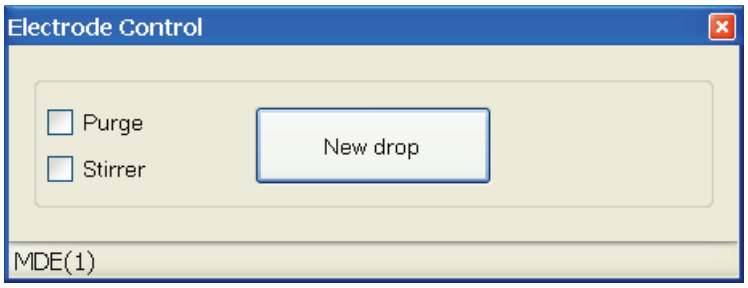


Figure 122 – The Electrode Control can be used switch purge and stirrer on or off and to create a new drop

Note: control of the MDE is also possible during a measurement using the Autolab control command. A specific MDE tab is available in the Autolab control window (see Figure 123). The Number of new drops controls the number of consecutive drops to knock off the mercury electrode.

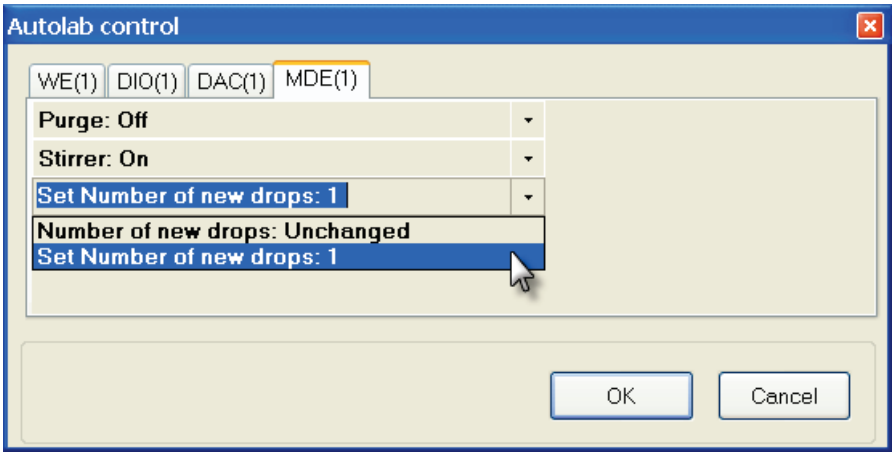


Figure 123 – Control of the MDE is possible through the Autolab control command

Manual control for MUX

Manual control over the MUX module is available from the View menu (see Figure 161).

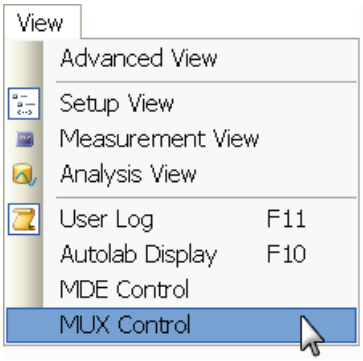


Figure 124 – Manual control of the MUX module is provided in the View menu

Through the MUX control it is possible to manually set one of the available MUX channel to active (see Figure 161).

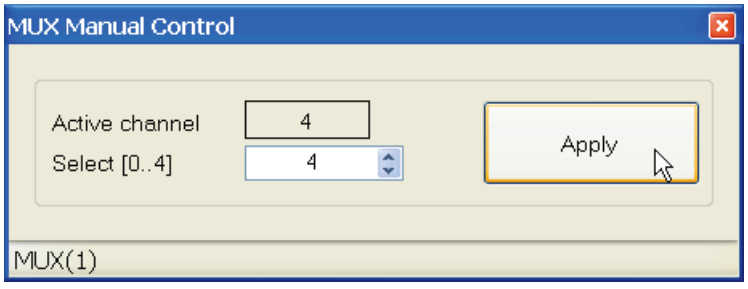


Figure 125 – The MUX Manual Control can be used to select one of the available MUX channels

Note: control of the MUX is also possible during a measurement using the Autolab control command (see Figure 126).

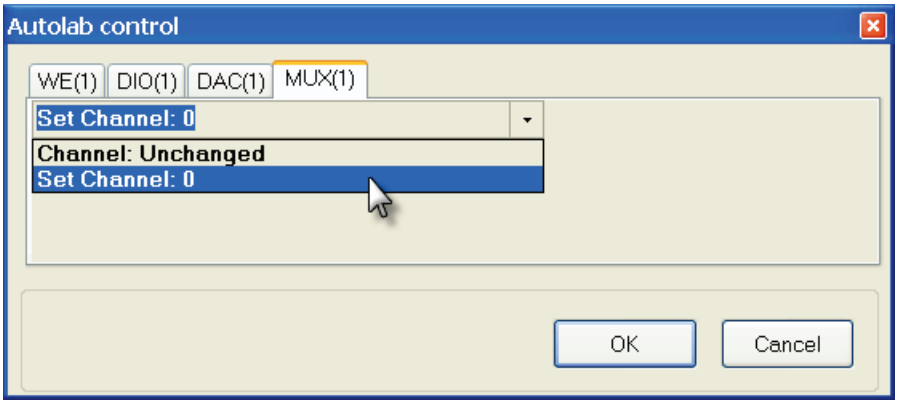


Figure 126 – Control of the MUX is also available in the Autolab control window

New Autolab control command

The Autolab control command has been redesigned and now displays the available properties under tabs. The number of available tabs depends on the hardware setup (see Figure 127).

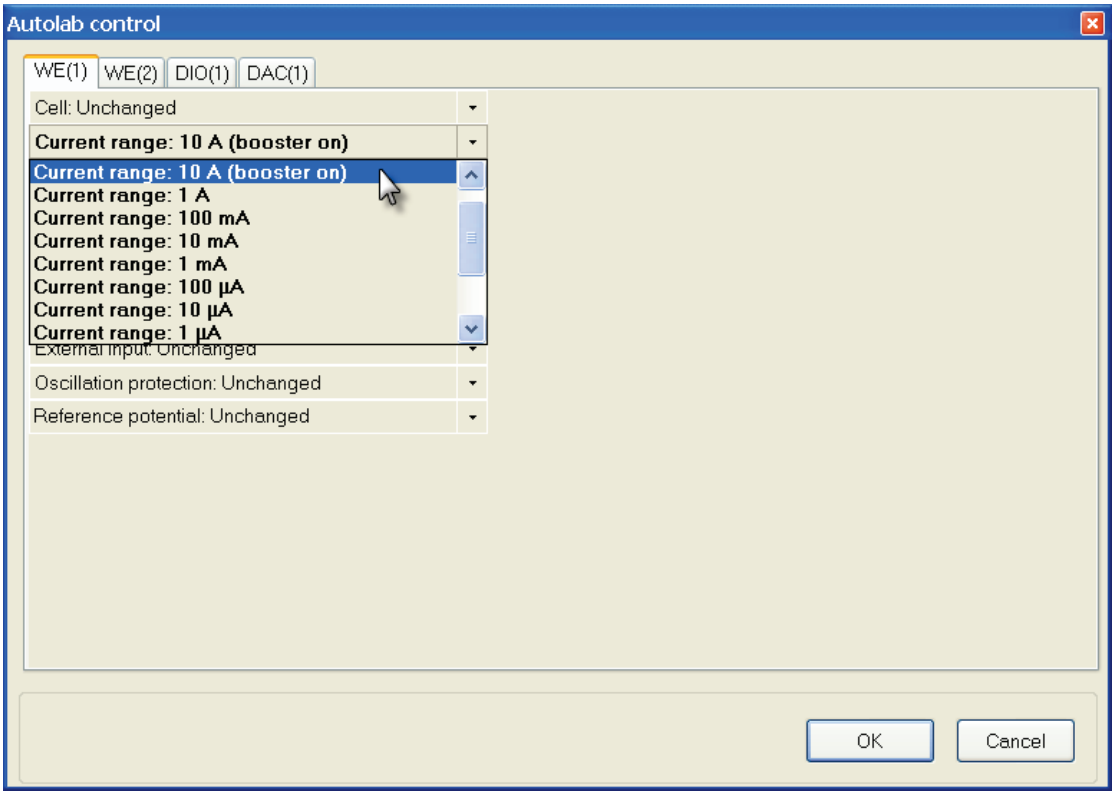


Figure 127 – The new Autolab control command

Note: more information about the Autolab control command can be found in the Autolab control tutorial.

Autolab display

The Autolab display, available from the View menu or through the F10 key has been modified. Two features have been added to the Autolab display:

Real-time display of Voltage and Current

The Autolab display can now be used to view the voltage and current values measured by the Autolab when no measurement is running (see Figure 128).

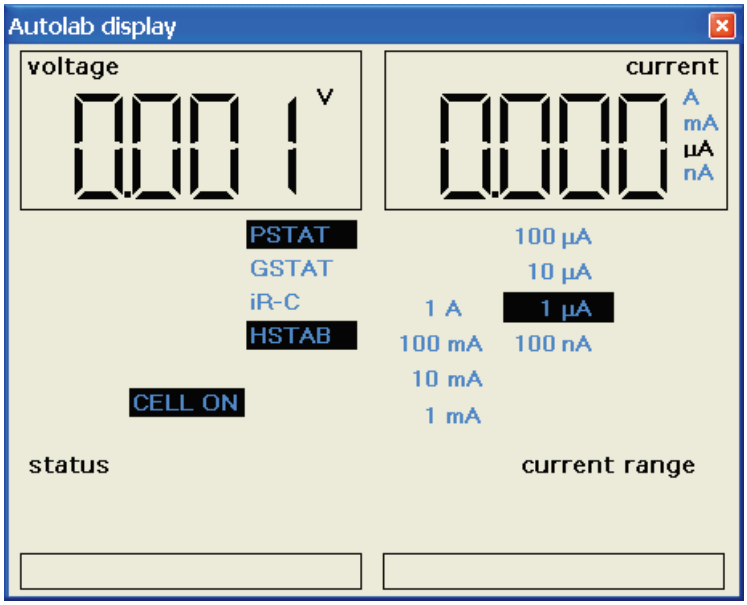


Figure 128 – The Autolab display can be used to view the voltage and current even if no measurement is running

Manual control of the instrument

The Autolab display can also be used to manually control the potential or the current of the Autolab. Depending on the instrument settings (PSTAT or GSTAT), it is possible to click the **voltage** or **current** label in the Autolab display to edit the value of the applied voltage or current applied on the electrochemical cell, respectively (see Figure 129).

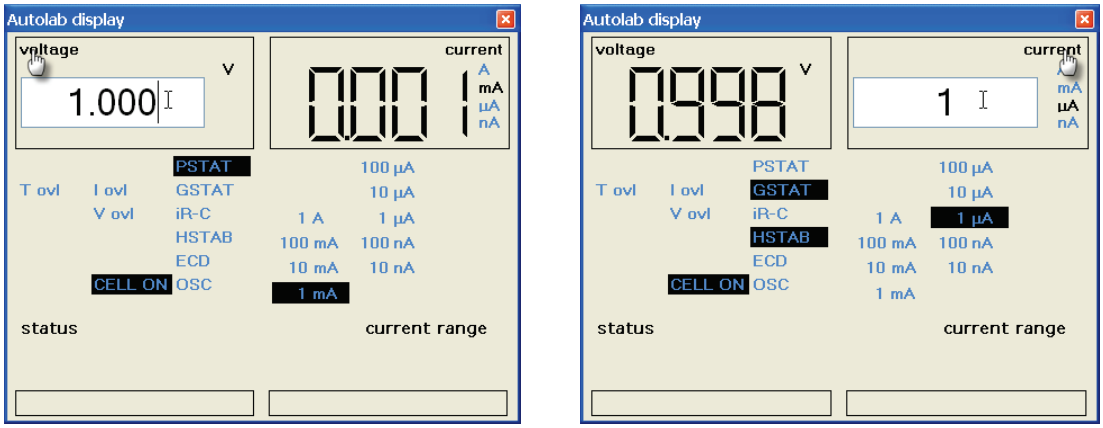


Figure 129 – Clicking the voltage label (left) or current label (right) in the Autolab display allows editing of the applied voltage or current

Skip button

The Skip button has been added to the toolbar. This button is active during a measurement and can be used to interrupt the currently executed command in the procedure and immediately move on to the next command.

Note: the Skip button does not change the settings of the Autolab. The instrument will remain in the settings encountered immediately before the skip button is pressed.

Reverse button

Nova now provides an additional button in the Autolab display that can be used to reverse the scan direction of linear sweep and cyclic staircase voltammetry commands (see Figure 130). This button is available both in potentiostatic and in galvanostatic mode.

Note: the Reverse button is not available for cyclic voltammetry measurements performed using the linear scan generator module (SCANGEN or SCAN250) and for the Voltammetric analysis commands.

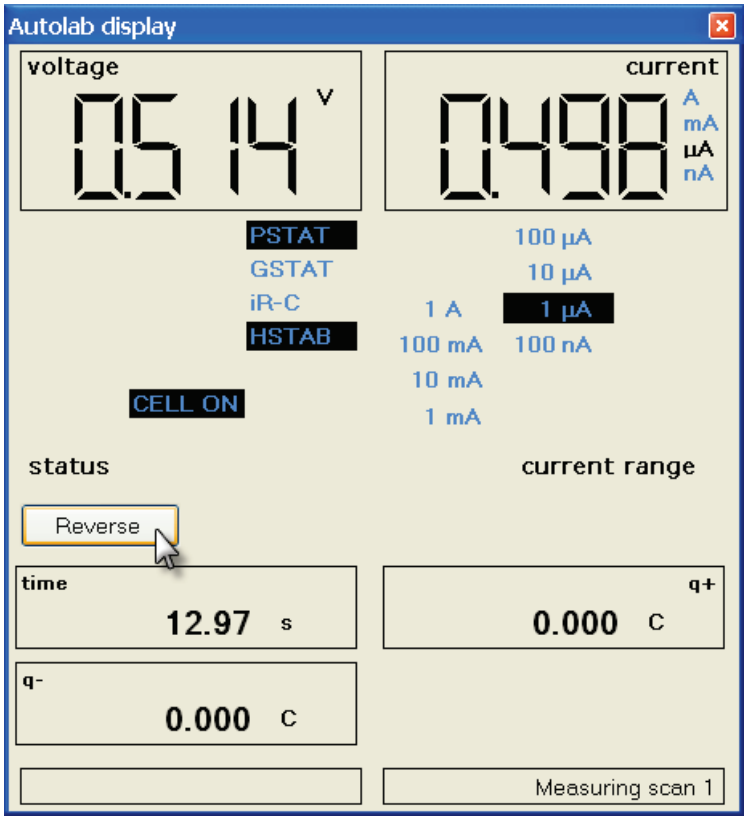


Figure 130 – The reverse button is now available in the Autolab display

Multiple plots in measurement view

This version of NOVA introduces the possibility of displaying up to 4 plots at the same time in the measurement view. Each plot can be configured independently and can be used to display measured data points or results from data handling commands or calculations. During the experiments, it is possible to change the arrangement of the plots using dedicated toolbar buttons (see Figure 131).

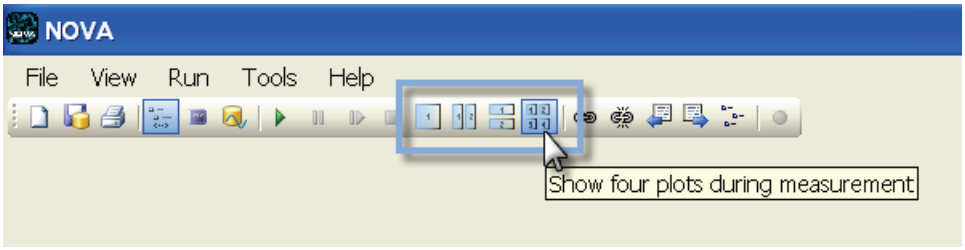


Figure 131 – The dedicated toolbar buttons for multiple plots

An example of the use of the multiple plot option is displayed in Figure 132.

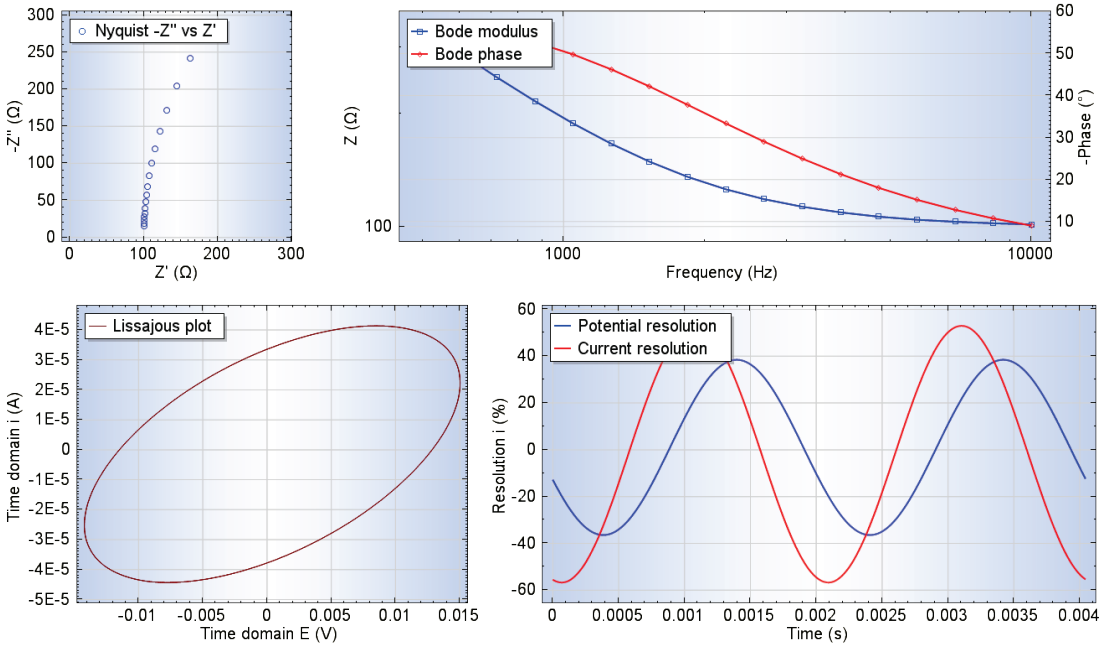


Figure 132 – Using the multiple plot feature in an impedance measurement: plot 1 (top left) - Nyquist plot, plot 2 (top right) - Bode plot, plot 3 (bottom left) - Lissajous plot, plot 4 (bottom right) - Resolution vs time

Note: results of calculations and data handling commands are displayed after the data has been collected.

Additionally, it is possible to copy plots from the analysis view into any of the 4 available plots in the measurement view. This provides the possibility to create overlays between data points being recorded real-time and data points from previous experiments (see Figure 133).

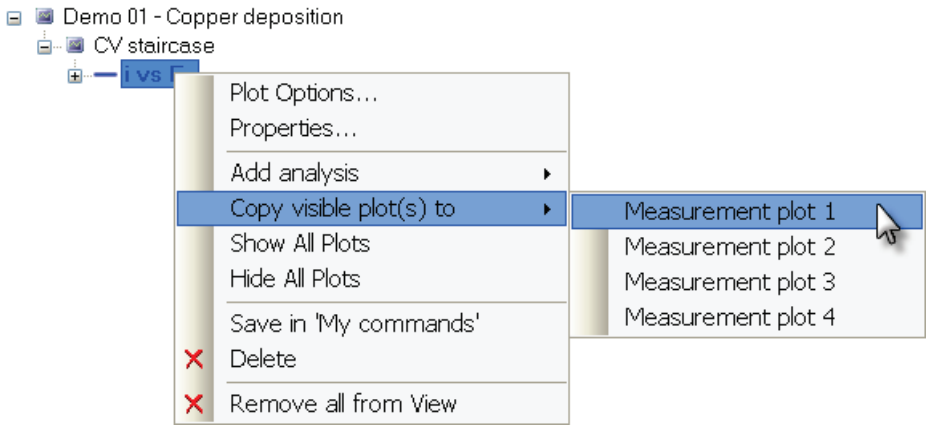


Figure 133 – Copying visible plots from the analysis view to the measurement view can be done by right-clicking a plot in the analysis view and choosing the location of the plot in the measurement view

Note: this option creates an exact copy of the selected plot(s), including any additions to the plot(s).

Send email

It is now possible to send an email, using a dedicated command, during an experiment (see Figure 134). This feature can be used to inform the user about the progress of a measurement when the experiments is very long.

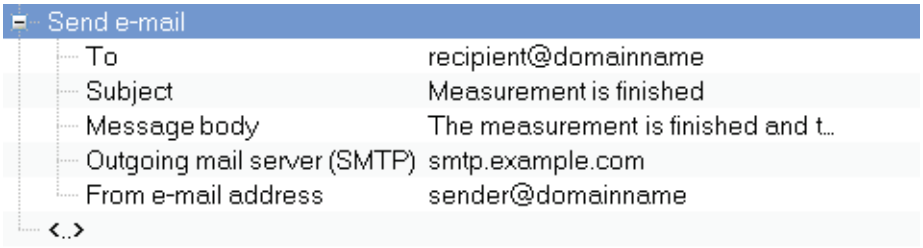


Figure 134 – It is now possible to send emails during an experiment

Check for update

An online check option is available from the Help menu (see Figure 135 and Figure 136). This option can be used to verify if a new version of NOVA is available. This option requires an internet connection.

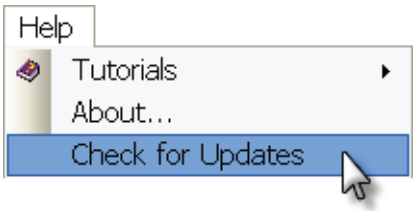


Figure 135 – Online check for updates

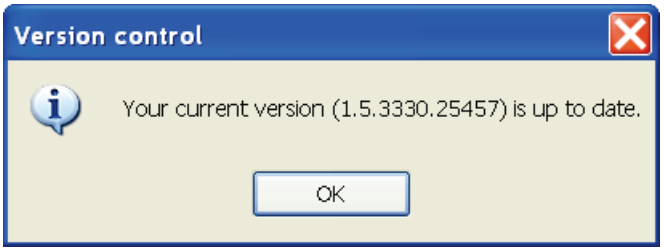


Figure 136 – The current version is up to date

If a new version is available, visit the www.metrohm-autolab.com website to download the update.

New data handling commands

Three new data handling commands have been added to the Data handling group of commands:

- Get array size
- Get array item
- Get first array item
- Get last array item

The get array size command can be used to determine the length of an array. When linked to an array of value, this command will return an integer which corresponds to the number of items in the array. Figure 137 shows a possible use for the Get array size command.

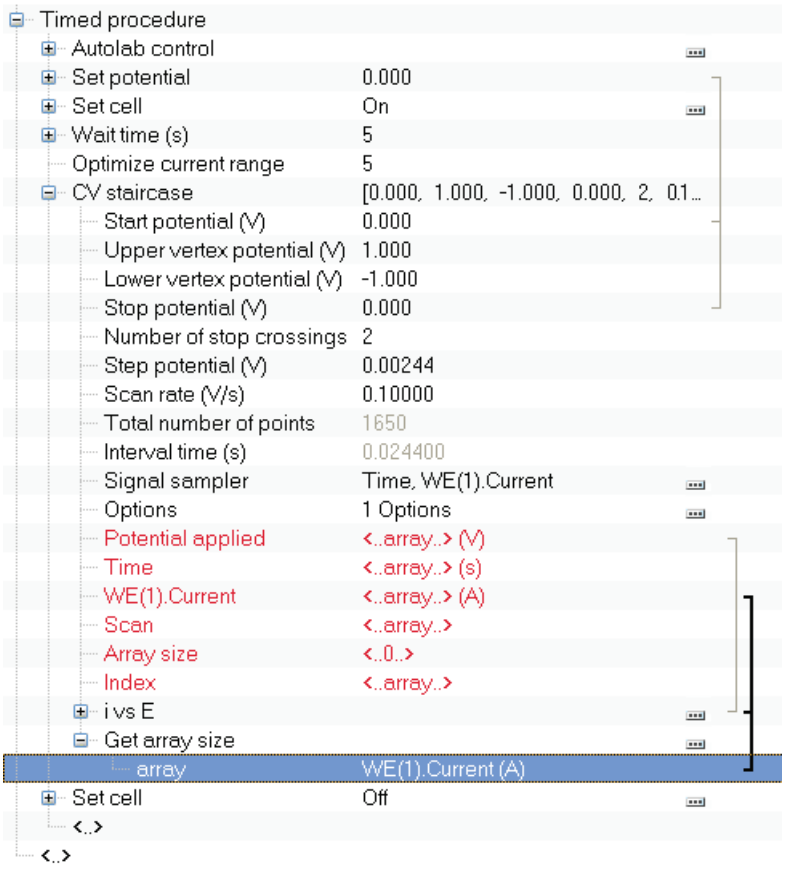


Figure 137 – The Get array size command used in combination with the CV staircase command

The total number of points parameter displayed in the CV staircase command is an estimation of the real number of data points. Depending on the scan rate and potential step, the real number of data points measured during by the CV staircase command could deviate slightly. The Get array size command can be used to determine the real number of data points.

The Get array item command can be used to extract the n^{th} value from an array while the Get last array item automatically looks for the last value in an array. Both commands can be used to extract specific values from a list of measured or calculated signals and use these values as parameters in the procedure.

Timed procedure in FRA frequency scan

It is now possible to add a Timed procedure to a FRA frequency scan. Commands located inside the timed procedure are executed for each frequency in the scan (see Figure 138).

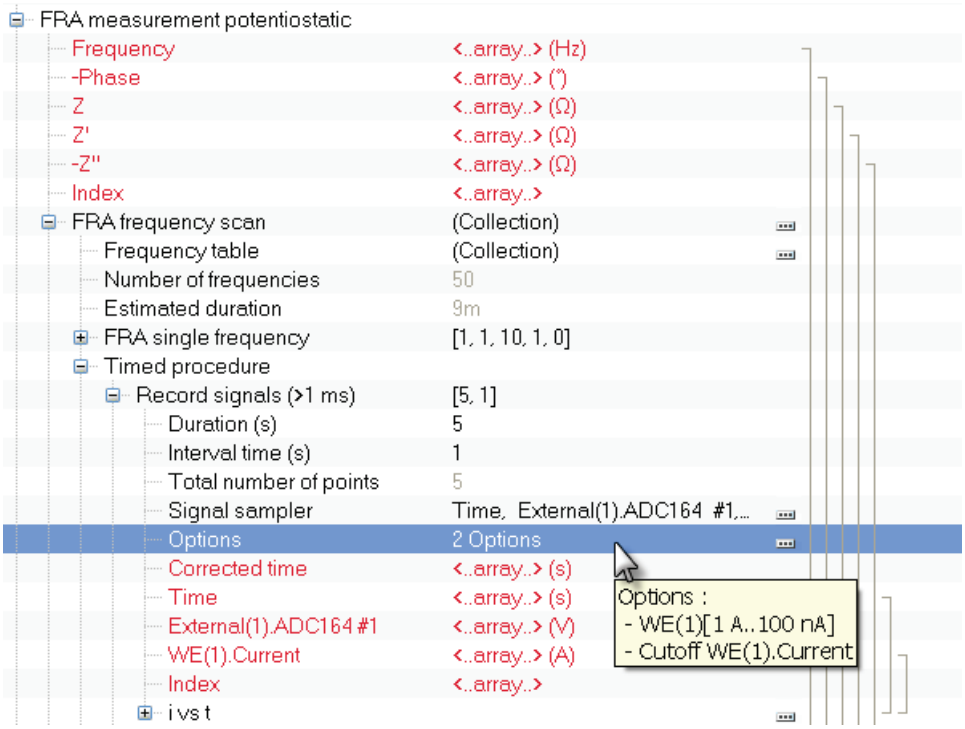


Figure 138 – Timed procedures can be added to the FRA frequency scan

This feature can be used to record external signals during a frequency scan or to test measured signals against a cutoff condition, as shown in Figure 138.

Note: the DSG of the FRA2 module is not switched off when the timed procedure is encountered. If required, it is possible to switch off the DSG input on the PGSTAT by using the Autolab control command in the timed procedure[7].

[7] Refer to the Impedance tutorial for more information and a practical example

New FRA commands

Two FRA commands have been added to the Measurement – impedance group of commands.

- FRA single frequency
- FRA single frequency (external)

These two commands are used in combination with the FRA frequency scan commands (potentiostatic, galvanostatic or external). When more than one FRA single frequency is added to a FRA frequency scan command, each frequency in the scan will be measured n times, where n is the number of FRA single frequency commands in the scan (see Figure 139).

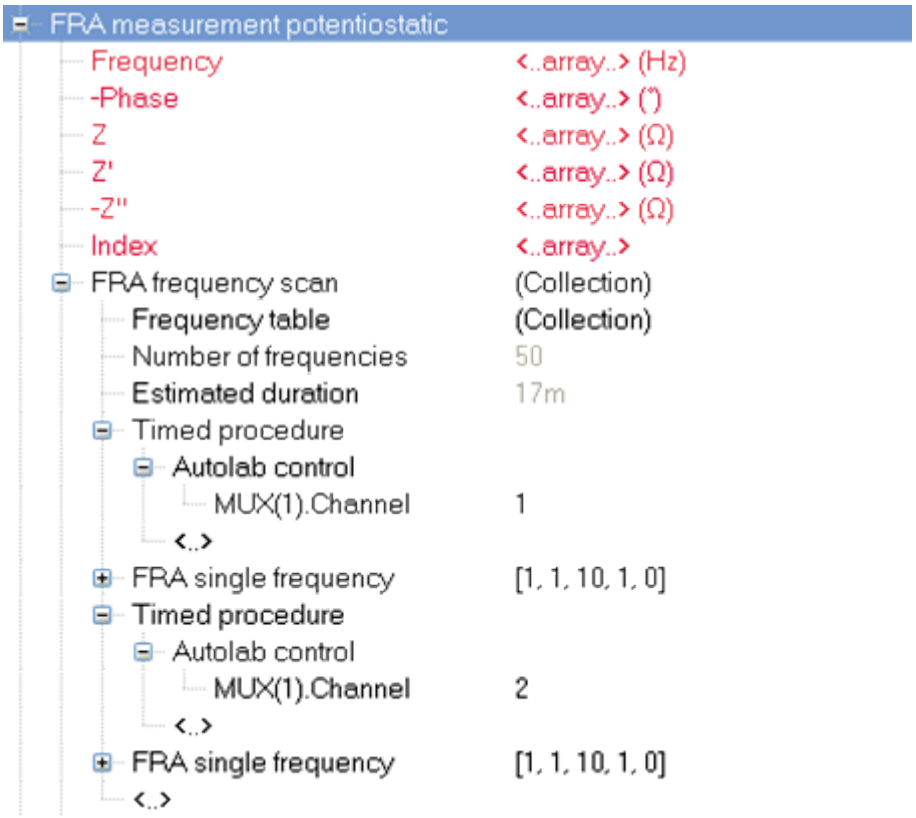


Figure 139 – Example of two FRA single frequency commands in a FRA measurement potentiostatic

Post measurement checks

The User log will now display messages after the measurement finishes advising to change the experimental condition, if applicable. The example shown in Figure 140 suggests changing the current range used in the measurement, as an overload was detected during the previous experiment.

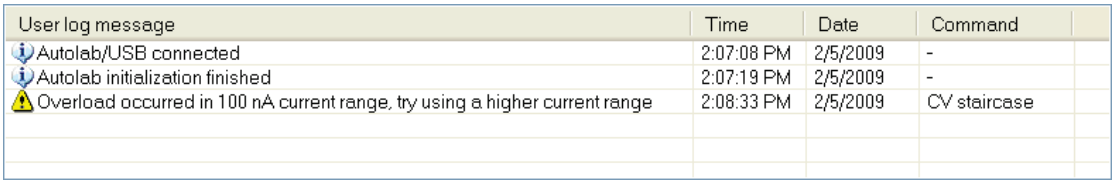


Figure 140 – Post measurement check

Note: it is possible to copy/paste the contents of the User log using the right-click menu.

Save data at the end of the measurement

By default, NOVA saves all the measured data points at the end of the experiment. It is now however possible to switch this feature off. This can be trough the options menu (see Figure 141).

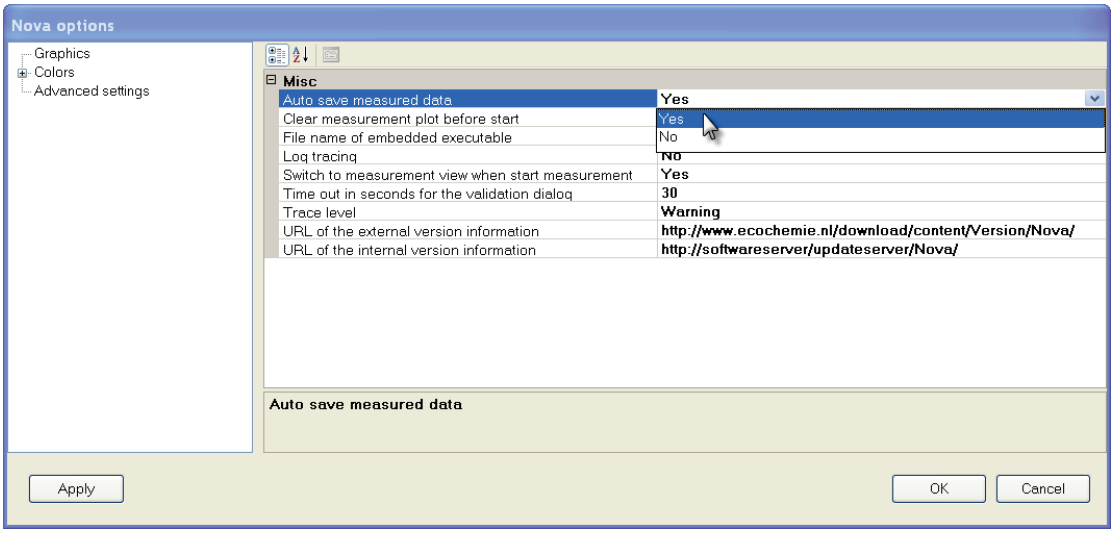


Figure 141 – The Automatic save feature can be switched on or off in the options menu

When this option is switched off, the user will be prompted at the end of each experiment to provide a name and a comment for the measurement. If the data is invalid or if saving the data is not required, an additional option to discard the measurement is provided (Figure 142).

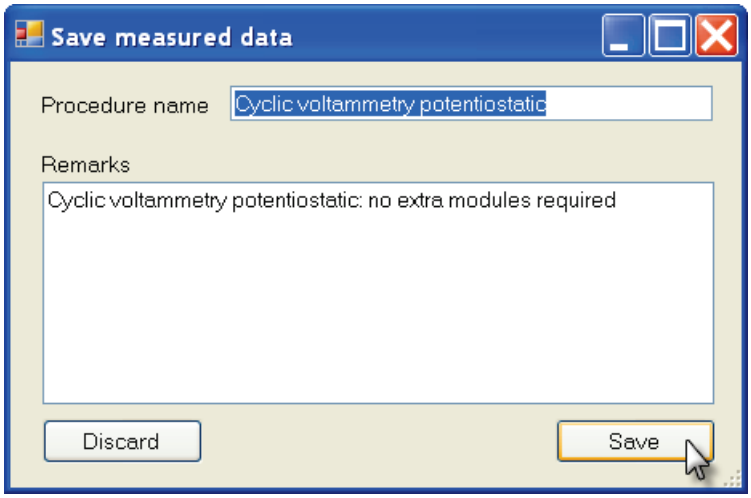


Figure 142 – When Automatic save is disabled, the user is prompted to specify name and remarks for the experiment. The user can also discard the data if it is invalid.

Note: pressing the Discard button will delete the measured data points immediately. These data points cannot be recovered.

Version and hardware overview in the About menu

The Help – about menu now displays extensive version and hardware configuration information (see Figure 143).

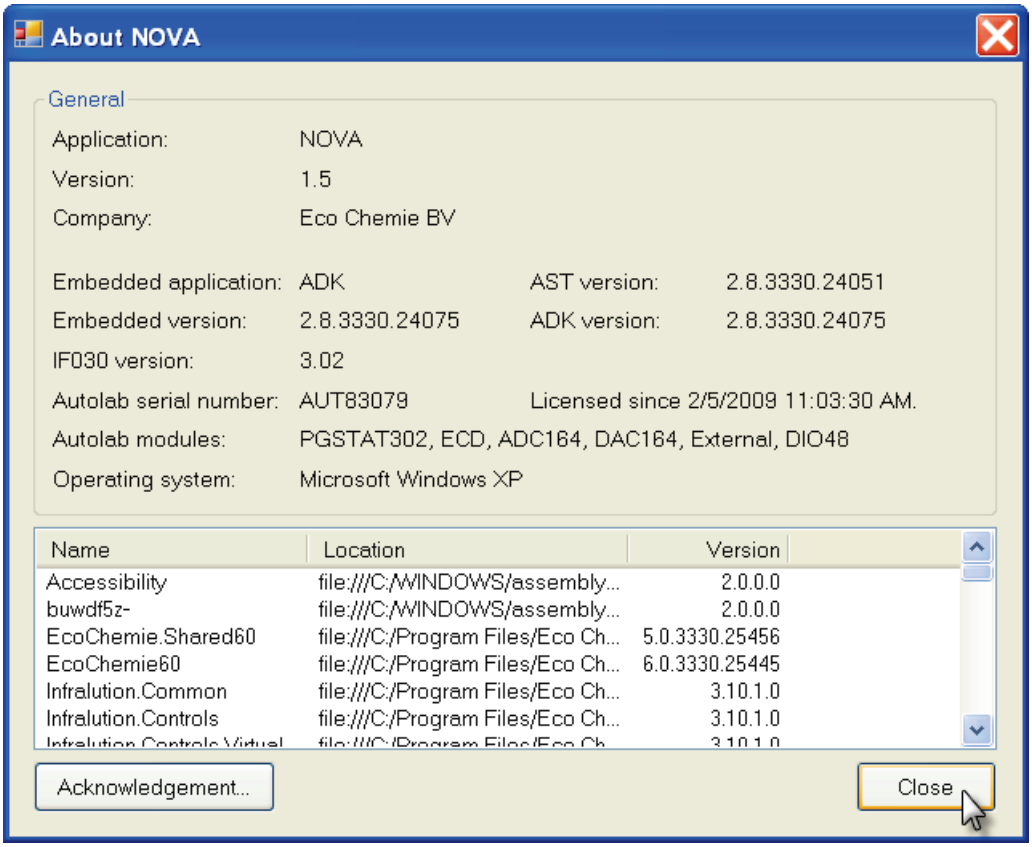


Figure 143 – The hardware configuration is now shown in the About menu, alongside software version information

Improved support for Metrohm devices

Support for Metrohm devices has been improved in this version of NOVA. The Initialization commands now have a dedicated interface in which the parameters of the device can be easily entered. Figure 144 shows the case of the Dosino settings interface.

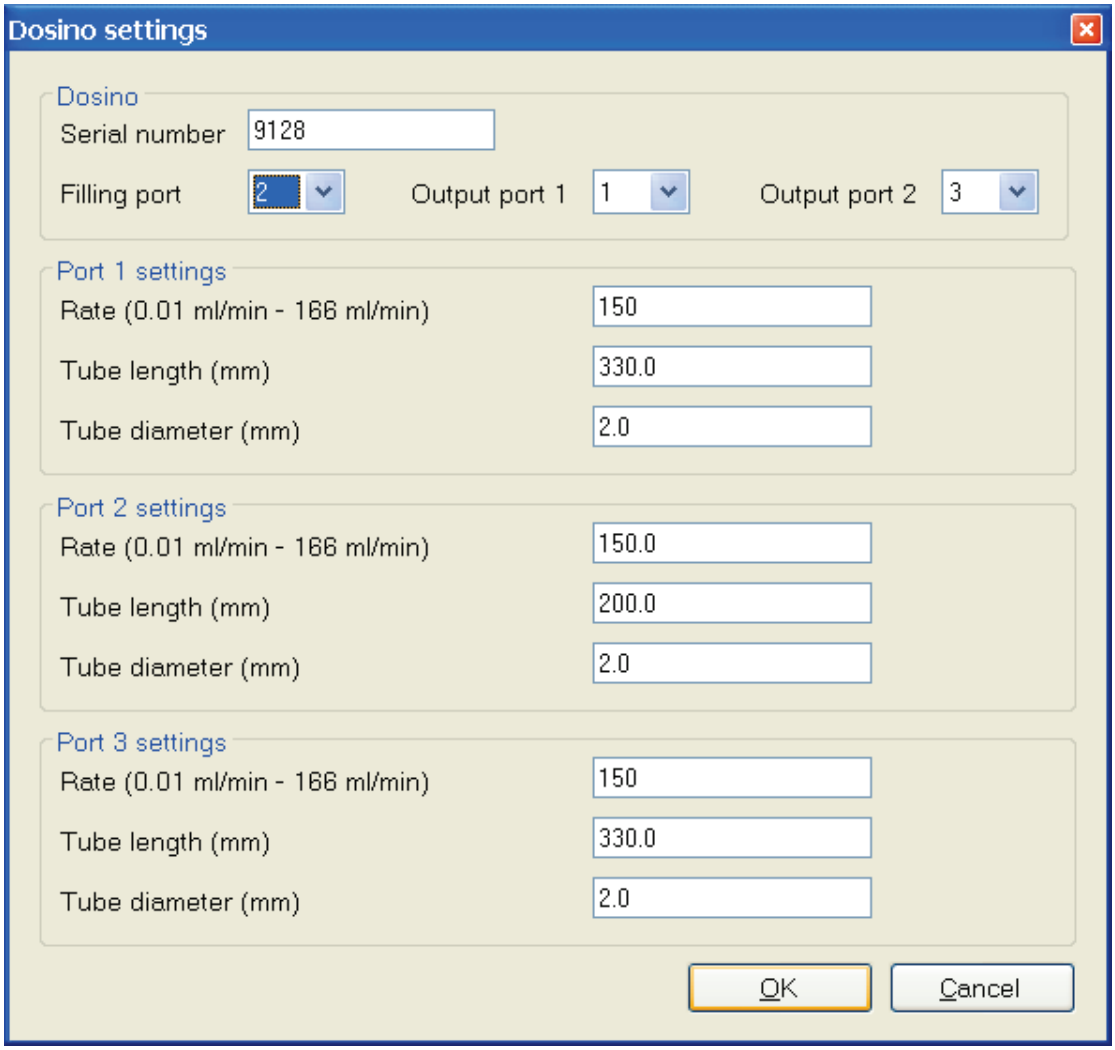


Figure 144 – Dosino settings interface

Autolab control in the options

The Options menu has been extended with an additional tab, which can be used to set specific Autolab settings at the end of each sampling step (see Figure 145). This can be used, for example, to create a new drop after each sampling step in sampled DC polarography.

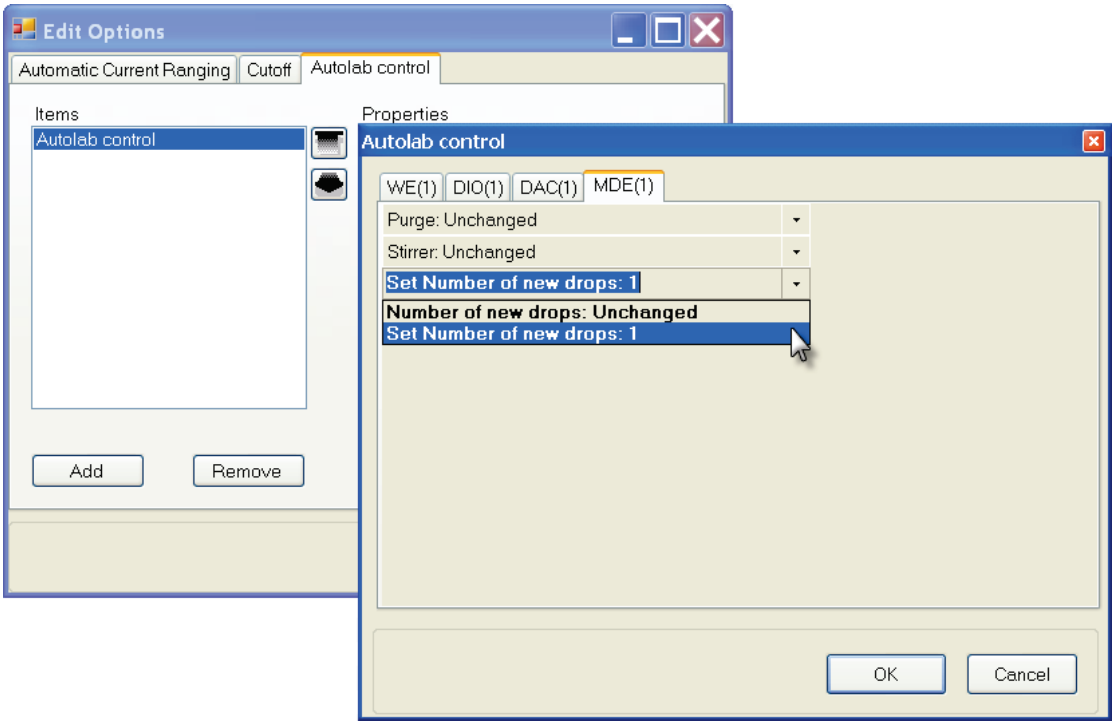


Figure 145 – The Autolab control command is now available in the options

Wait for DIO trigger

A wait for DIO trigger command has been added to the Measurement – General group of commands. With this command, it is possible to force the procedure to hold until a predefined DIO trigger is detected on one of the DIO connectors of the Autolab (see Figure 146).

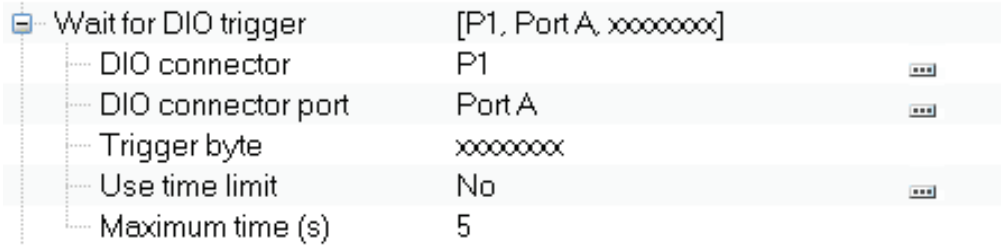


Figure 146 – The Wait for DIO trigger command is now available for receiving triggers

For the trigger byte, it is possible to define the sequence using 1 (pin up), 0 (pin down) or x (wildcard). Additionally, it is possible to define a maximum time limit for the command. If the predefined sequence is not detected within the time limit, the measurement will continue[8].

While the software is waiting for the DIO trigger, the current connector status is displayed in the lower right corner of the Autolab display (see Figure 147).

[8] More information on DIO triggers can be find in the External devices tutorial

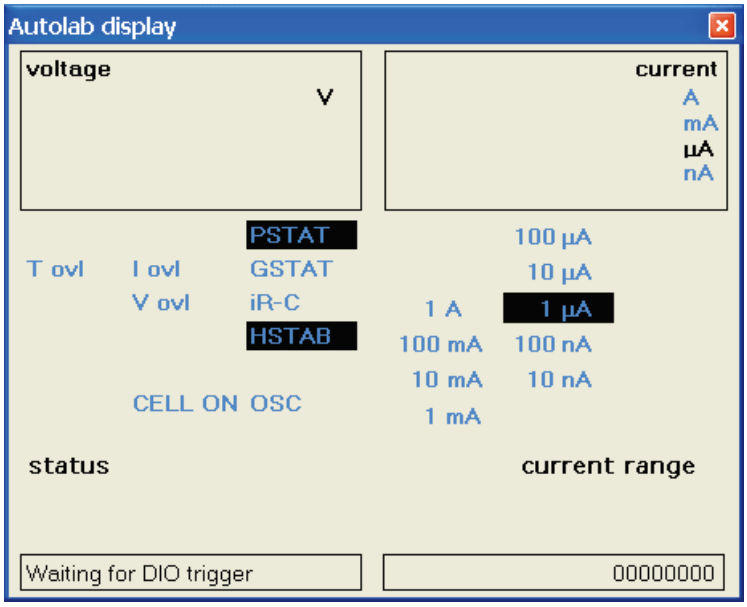


Figure 147 – The DIO status is displayed in the lower right corner when waiting for a trigger

Note: the DIO connector status is verified with an interval time of 100 ms.

Changes to the Autolab procedures

The following default procedures have been added to the Autolab group in the setup view:

- Linear sweep voltammetry potentiostatic
- Linear sweep voltammetry galvanostatic
- Differential pulse voltammetry
- Square wave voltammetry
- Sampled DC polarography
- Chrono amperometry high speed
- Chrono potentiometry high speed

The following Autolab procedures have been renamed for clarity purpose:

- Cyclic voltammetry linear scan, previously called *Linear scan*
- Cyclic voltammetry linear scan high speed, previously called *High speed linear scan*
- Chrono amperometry ($\Delta t > 1$ ms), previously called *Chrono amperometry*
- Chrono potentiometry ($\Delta t > 1$ ms), previously called *Chrono potentiometry*

The following Autolab procedures have been removed from the list:

- Cyclic voltammetry with EQCM
- Cyclic voltammetry with BA
- Cyclic voltammetry with ECD

Specific instructions on how to use these three modules are provided in the tutorials.

Autolab test procedures

Special procedures are now included in a special *Module test* database installed with NOVA. These procedures can be used to test specific hardware module and the Autolab potentiostat, using the Autolab dummy cell (see Figure 148).

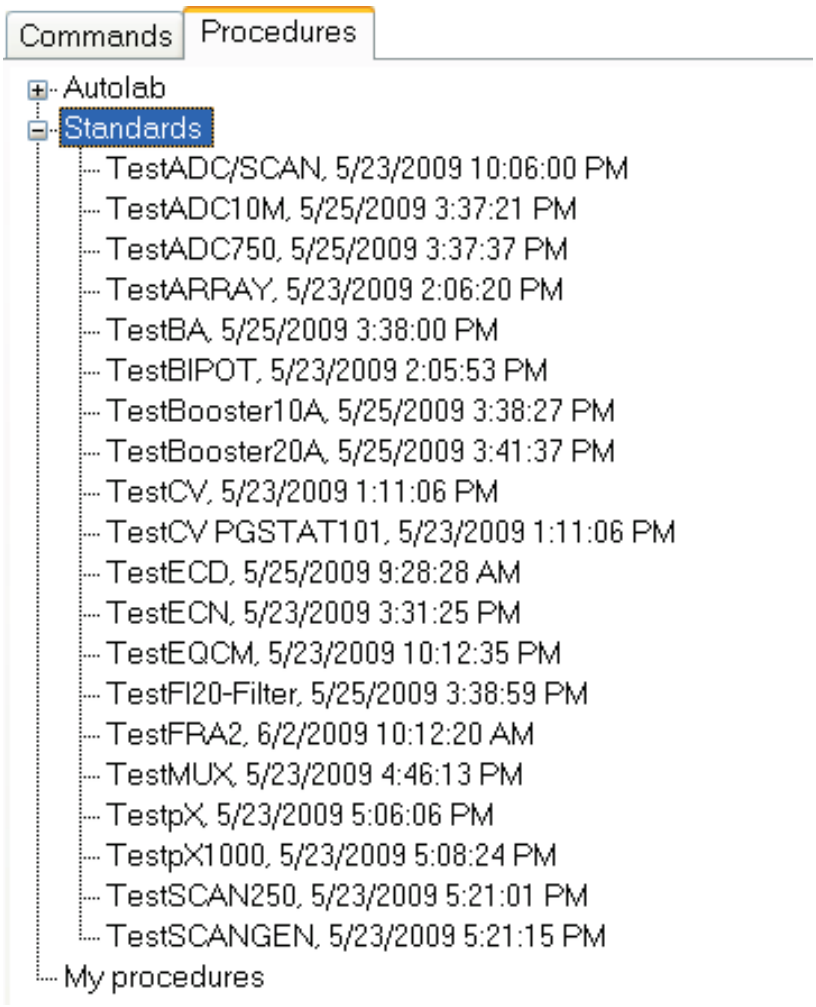


Figure 148 – Module test procedures are now included in the software

More information can be found in the *Module test with Nova* document, available from the Help menu.

PGSTAT101 support

Figure 149 – The new Autolab PGSTAT101

Instrument specifications

The PGSTAT101, shown in Figure 149, is a potentiostat/galvanostat with USB interface. The specifications of the device are listed below:

- Compliance voltage: 10 V
- Maximum applied potential: 10 V
- Maximum current: 100 mA
- Electrode connections: CE, RE, S, WE and additional analog ground
- Analog I/O[9]: E_{out}, i_{out}, V_{in}, V_{out}
- Digital I/O: 8 outputs and 4 inputs
- Internal dummy cell: 100 Ohm + 1 MOhm // 1 µF
- iR compensation

[9] Requires optional I/O cable.

Hardware setup PGSTAT101

The new Autolab PGSTAT101 is now supported in the latest version of NOVA. The instrument can be selected in the hardware setup window (see Figure 150).

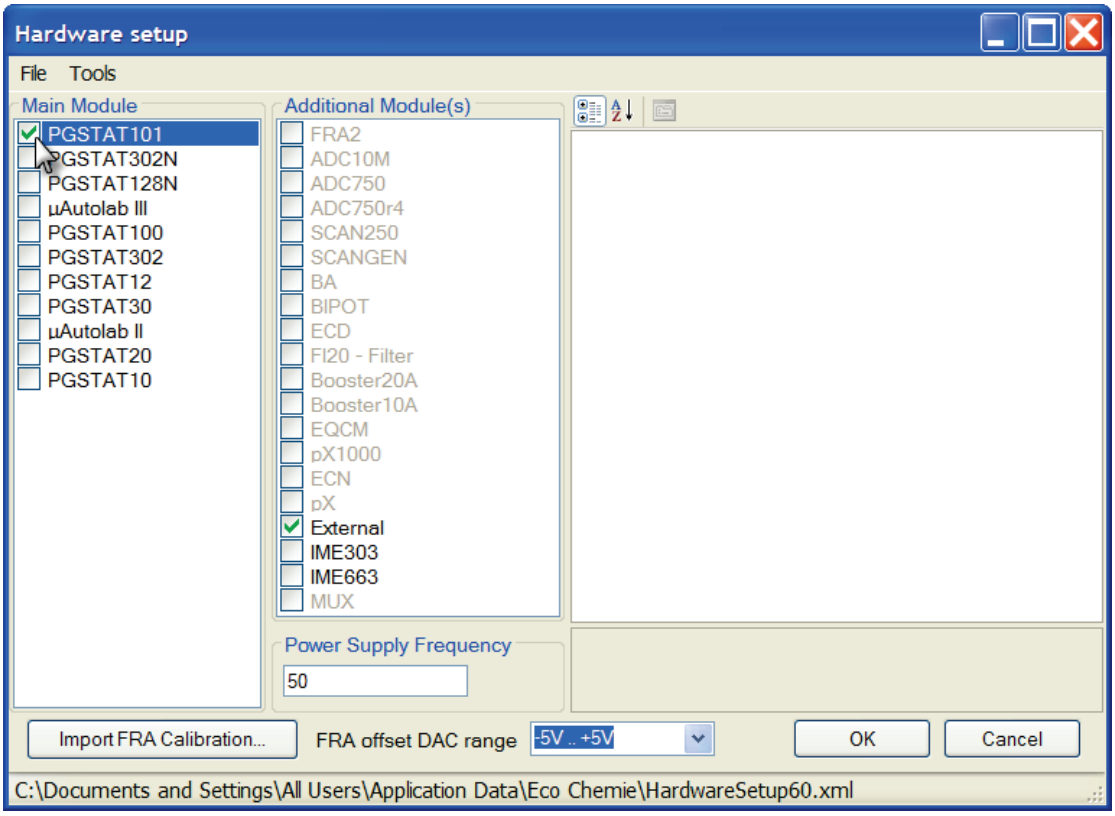


Figure 150 – The PGSTAT101 is available in the hardware setup

Note: the PGSTAT101 is not modular and no additional modules, except the IME663 and the IME303, can be selected when this instrument is used.

The PGSTAT101 can be fitted with the **optional** I/O cable. This cable provides four additional connections to the PGSTAT101 analog circuits (see Figure 151). All the signals are with respect to Autolab ground and indirectly to protective earth.

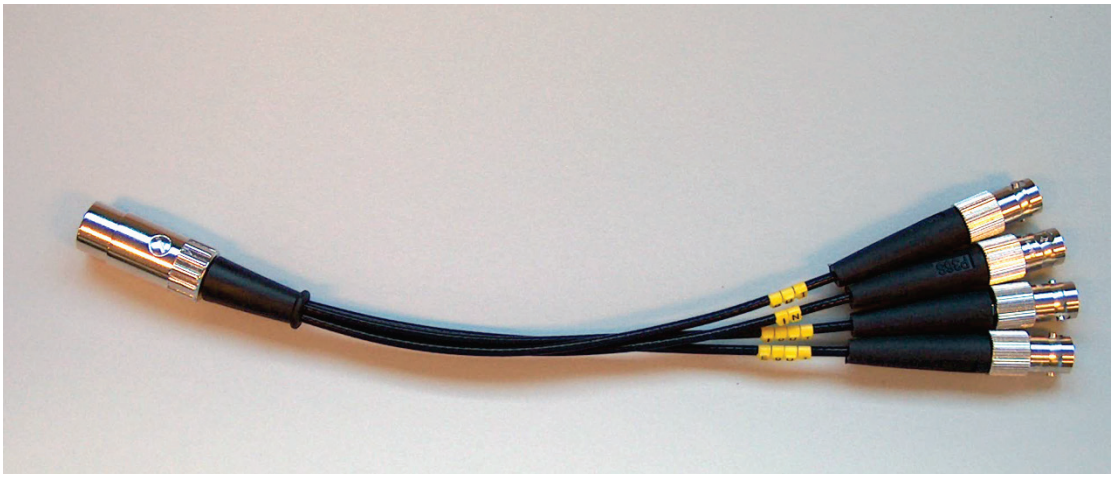


Figure 151 – The optional I/O cable for the PGSTAT101

With the optional I/O cable, the following signals are available:

E_{OUT} – This output corresponds to the differential potential of RE versus S[10]. The output voltage will vary between ±10 V.
i_{OUT} – This signal corresponds to the inverted output of the current-to-voltage converter circuit of the PGSTAT101[11]. A 1 V signal corresponds to {-1 x the selected current range}.
V_{OUT} – This output corresponds to the DAC output. It is controlled by software and is meant to be used to control external devices, like the rotating speed of a Rotating Disc Electrode (RDE). The output level varies between ±10 V.
V_{IN} – This input corresponds to the ADC input. This input can be used for measuring a second signal. The input range is ±10 V.

More information about the PGSTAT101 hardware can be found in the PDF version of the Getting started, available from the Help – Tutorials menu.

[10] The E_{out} value corresponds to -WE(1).Potential.
[11] The i_{out} value corresponds to -WE(1).Current/Current range.

Diagnostics

The diagnostics application has been adjusted and the PGSTAT101 has been added to the list of devices available in the test (see Figure 152).

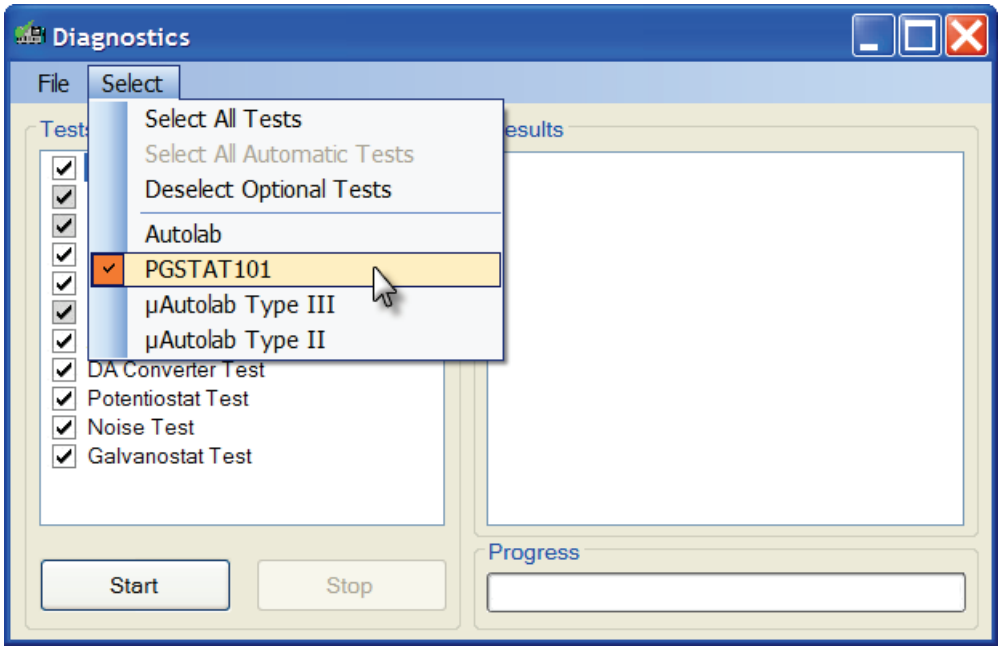


Figure 152 – The PGSTAT101 has been added to the list of devices in the diagnostics application

Note: the PGSTAT101 is equipped with an internal dummy cell. When the diagnostics tests are performed on this instrument, the reference (RE) and counter (CE) electrode leads must be connected together on one hand and the working (WE) and sense (S) electrode leads must be connected together on the other hand. Make sure that RE/CE and S/WE are not in contact. A reminder is shown at the beginning of the diagnostics (see Figure 153).

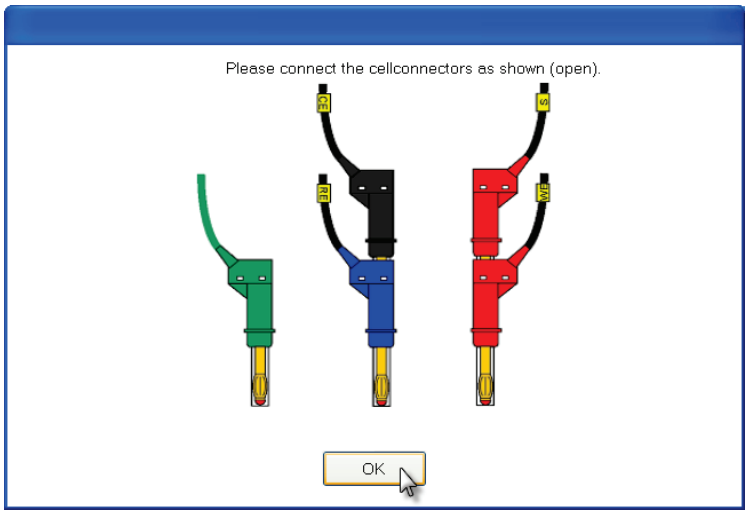


Figure 153 – When the diagnostics are performed with the PGSTAT101, connect RE to CE and S to WE as shown in the visual reminder

PGSTAT101 test

A specific procedure to test the PGSTAT101 has been added to the Module test database (default location: *C:\Program Files\Eco Chemie\Nova 1.5\Shared Databases\Module test*). This test procedure can be used to verify the basic functionality of the instrument. The test is performed on the internal dummy cell. Refer to the Module test documentation for more information (available from the Help – Tutorials menu).

Maximum current

The highest current range available in the PGSTAT101 is 10 mA. This current range has a linearity of 10 times, which means that a maximum of 100 mA can be applied to the cell in galvanostatic mode and that a maximum of 100 mA can be measured in this current range, in potentiostatic mode.

To apply 100 mA in GSTAT mode, the offset value must first be set to 50 mA, using the Autolab control command (see Figure 154).

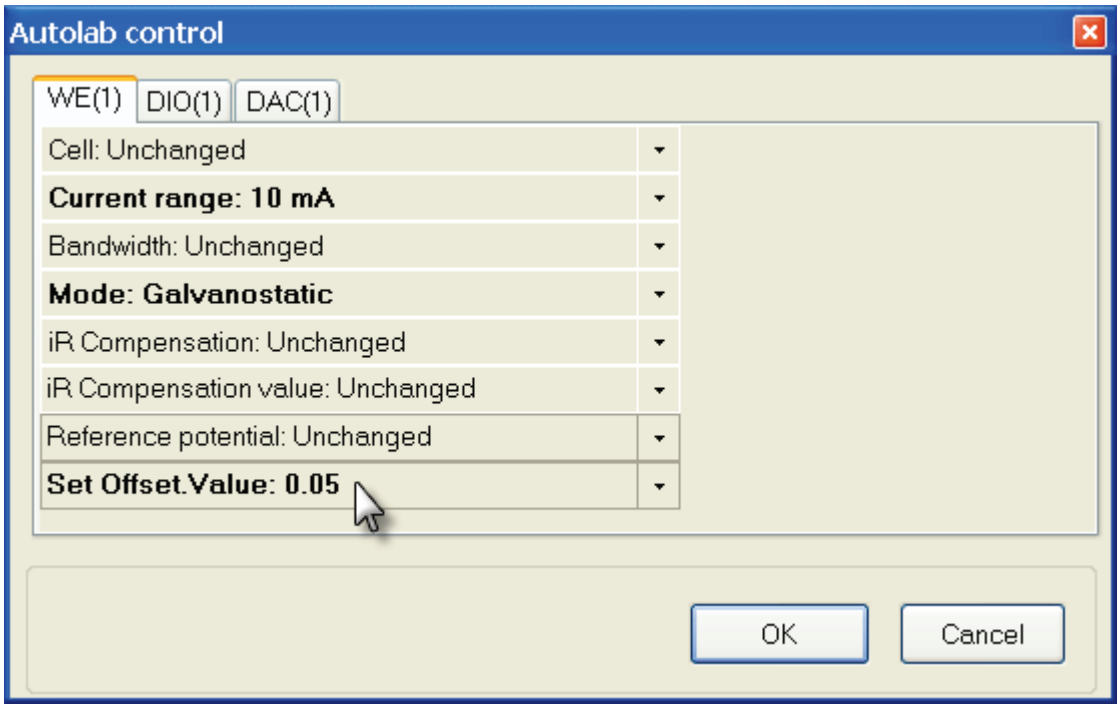


Figure 154 – The offset value must be set to 50 mA in order to apply 100 mA in the 10 mA current range

Autolab control

The Autolab control command has been adjusted for the PGSTAT101 (see Figure 155).

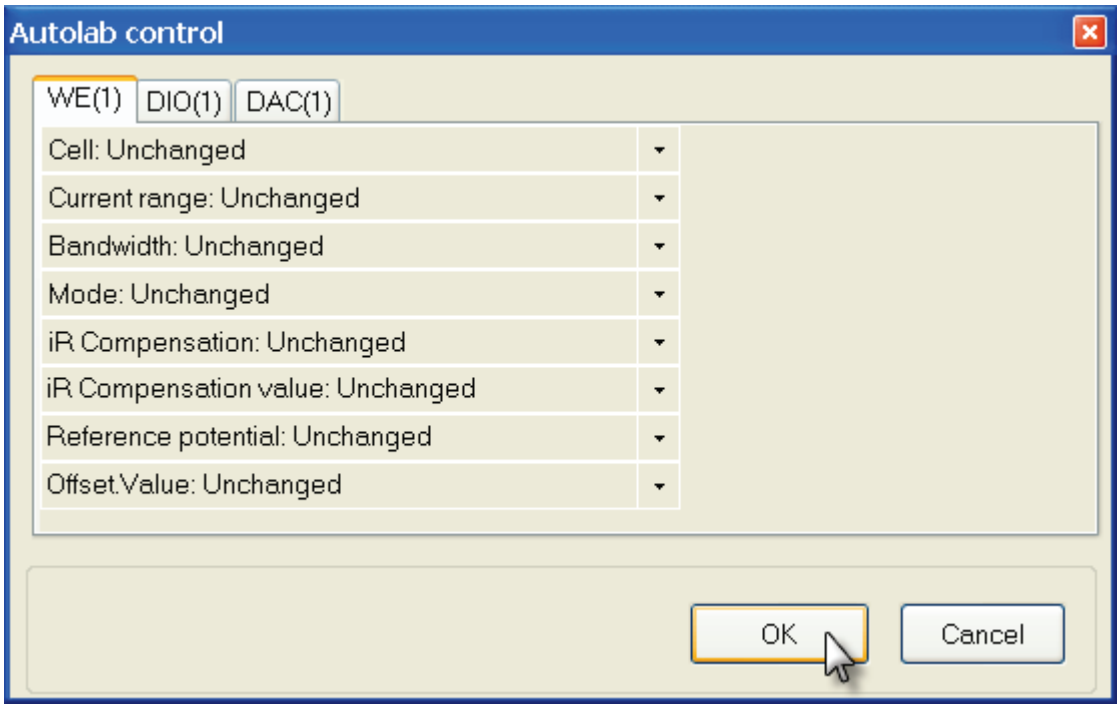


Figure 155 – The Autolab control window has been adjusted for the PGSTAT101

TTL triggering

The PGSTAT101 is fitted with a single, non configurable DIO connector. The DIO connector has a total of eight write lines and four read lines (see Figure 156).

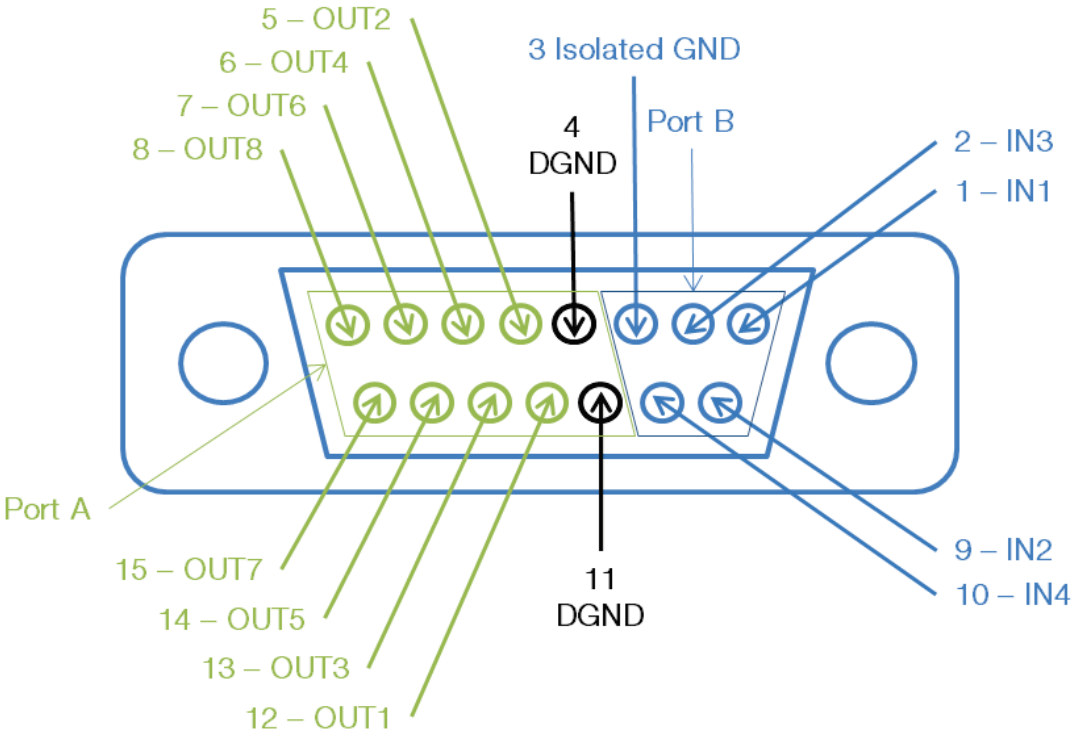


Figure 156 – Mapping of the PGSTAT101 DIO connector

Note: Port A includes 8 write lines and two digital ground pins (pin 4 and pin 11). Port B includes 4 read lines and an isolated ground pin (pin 3). All pins on Port B are galvanically isolated. Do not use pin 4 or pin 11 as ground pin for the read lines.

Important: the write lines of the PGSTAT101 DIO connector are capable of supplying a maximum current of 200 mA. Suitable pull-down resistors should be placed in the write lines of the DIO cable connected to the PGSTAT101. A typical value for the pull-down resistance is about 1 kΩ. Please refer to the user manual of the external device connected to the PGSTAT101 for more information.

The *Autolab control* command only shows a single option in the DIO tab, where the 8 write pins of the single DIO connector can be defined (see Figure 157).

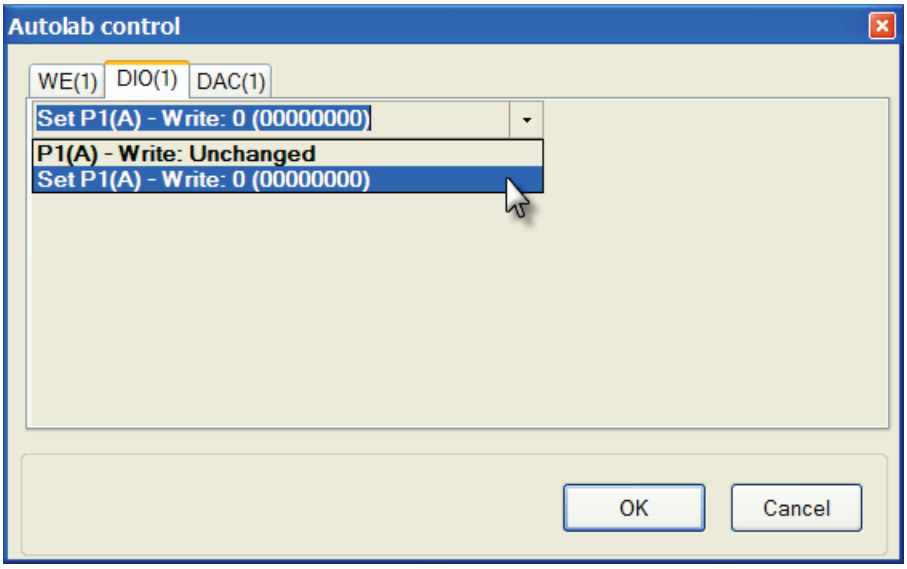


Figure 157 – The 8 pins of the write section of the single DIO port of the PSGTAT101 can be set directly from the Autolab control command

The *Wait for DIO trigger* command, available in the Measurement – General group of command has also been adjusted. Pressing the ... button in the procedure editor opens a dialog window which can be used to identify the available connectors and ports for the instrument in use. For the PGSTAT101, a single input port is available on the DIO connector (see Figure 158).

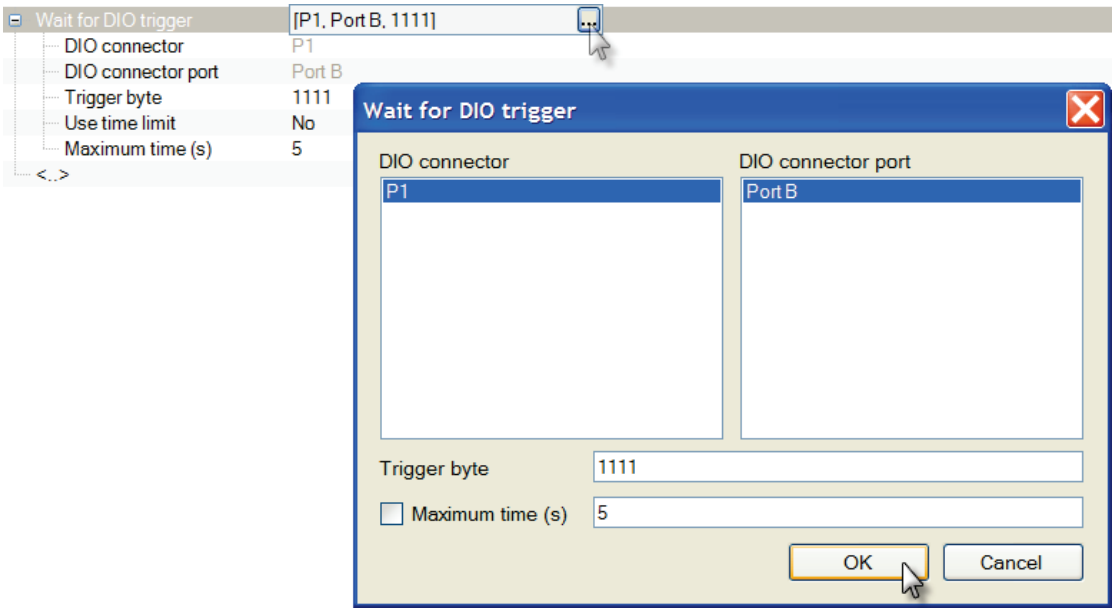


Figure 158 – The new Wait for DIO trigger interface

Note: the trigger byte consists of 4 bits for the PGSTAT101.

NOVA 1.4 Release notes (Released 14/09/2008)

Introduction

These notes provide an overview of the new features introduced in NOVA 1.4 compared to the previous release.

The following items have been added to NOVA 1.4:

- A new set of tutorials, available from the Help menu

- Support for the modules

  - pX1000
  - EQCM
  - ECD

- Support for the instruments

  - PGSTAT20
  - PGSTAT128N

- Improvements and additions

  - Tutorials
  - Simplified user interface
  - New Autolab procedures
  - Grouped commands
  - Procedure templates
  - New plotting framework
  - Installed on same computer as previous releases
  - DAC control in Autolab control
  - Cutoffs
  - Simplified FRA frequency range editor
  - FRA Galvanostatic support
  - pH calibration
  - Data repository
  - Reverse compatibility with previous NOVA versions
  - New data analysis framework and data analysis tools
  - New data handling and new data analysis commands
  - My commands
  - Improved Import GPES command
  - Import and Export ASCII
  - G circuit element in Fit and Simulation
  - Kronig-Kramers calculation
  - Metrohm liquid handling support
  - External devices control

Tutorials

A series of short tutorials is available from the Help menu in Nova (see Figure 159). Each tutorial is dedicated to a specific measurement technique or aspect of the software.

Some tutorials include procedures that can be used to perform simple measurements on the Autolab dummy cell.

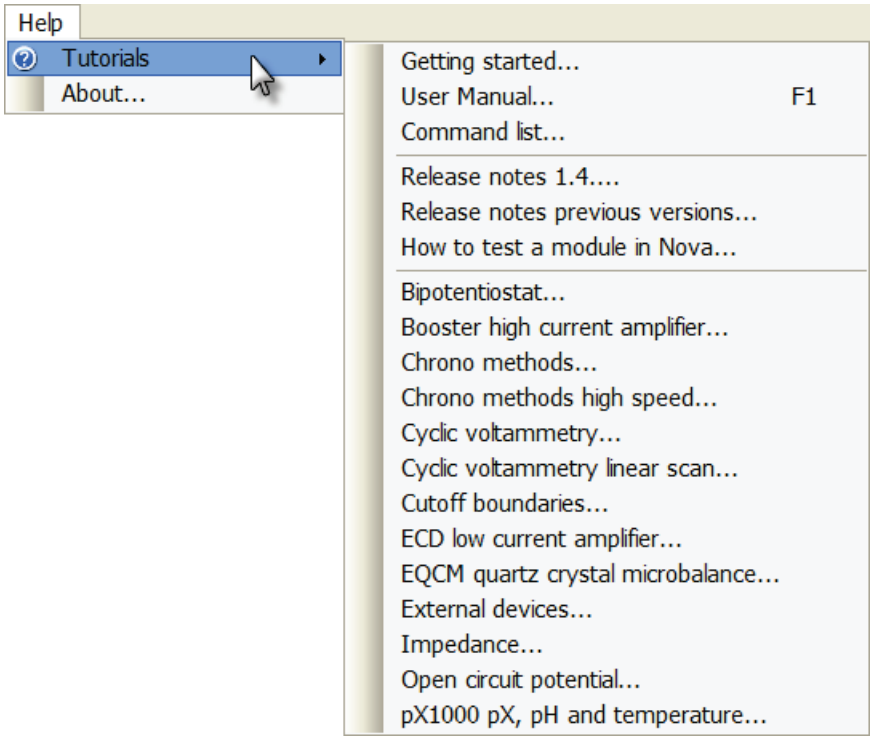


Figure 159 – A series of short tutorials is available from the Help menu

Modules support

NOVA 1.4 introduces the support for the ECD, pX1000 and EQCM modules.

Hardware support

The hardware setup of NOVA 1.4 now includes the PGSTAT128N and PGSTAT20[12] (see Figure 160).

[12] With serial number > 960350.

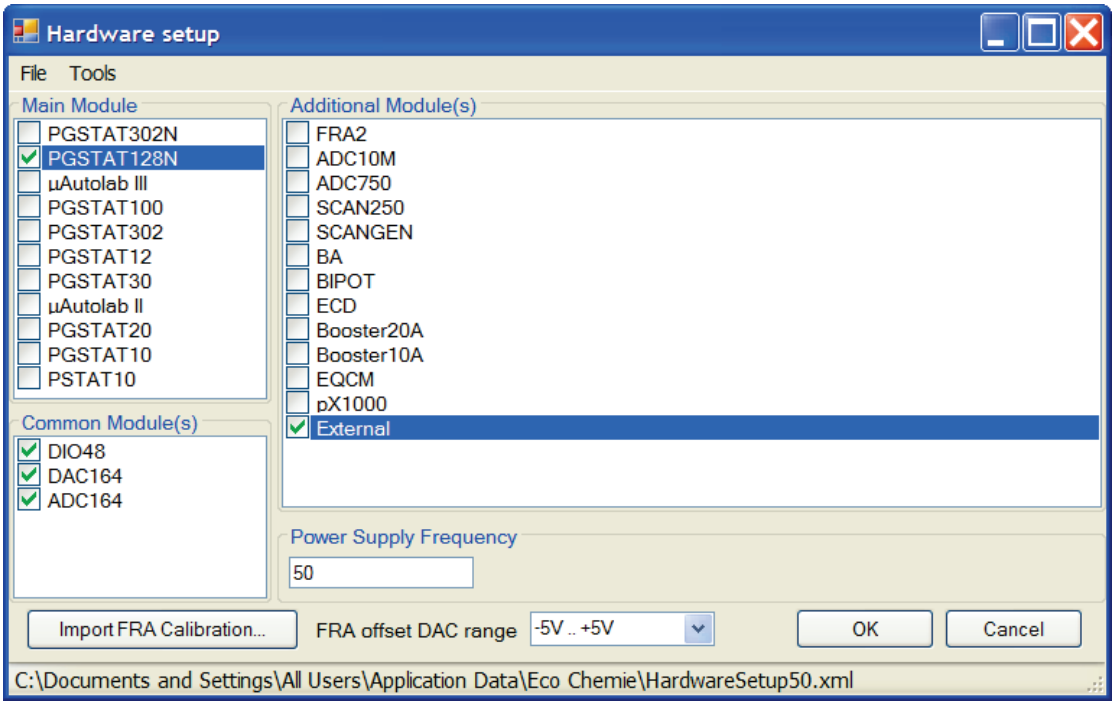


Figure 160 – The hardware setup window

Simplified user interface

NOVA 1.4 introduces a lighter user interface. A number of commands have been condensed into one-line commands. Figure 161 shows the factory default Cyclic voltammetry procedure. The Autolab control, Set Cell, Wait time and Optimize current range command have been reduced to a single line in the procedure editor (see Figure 161).

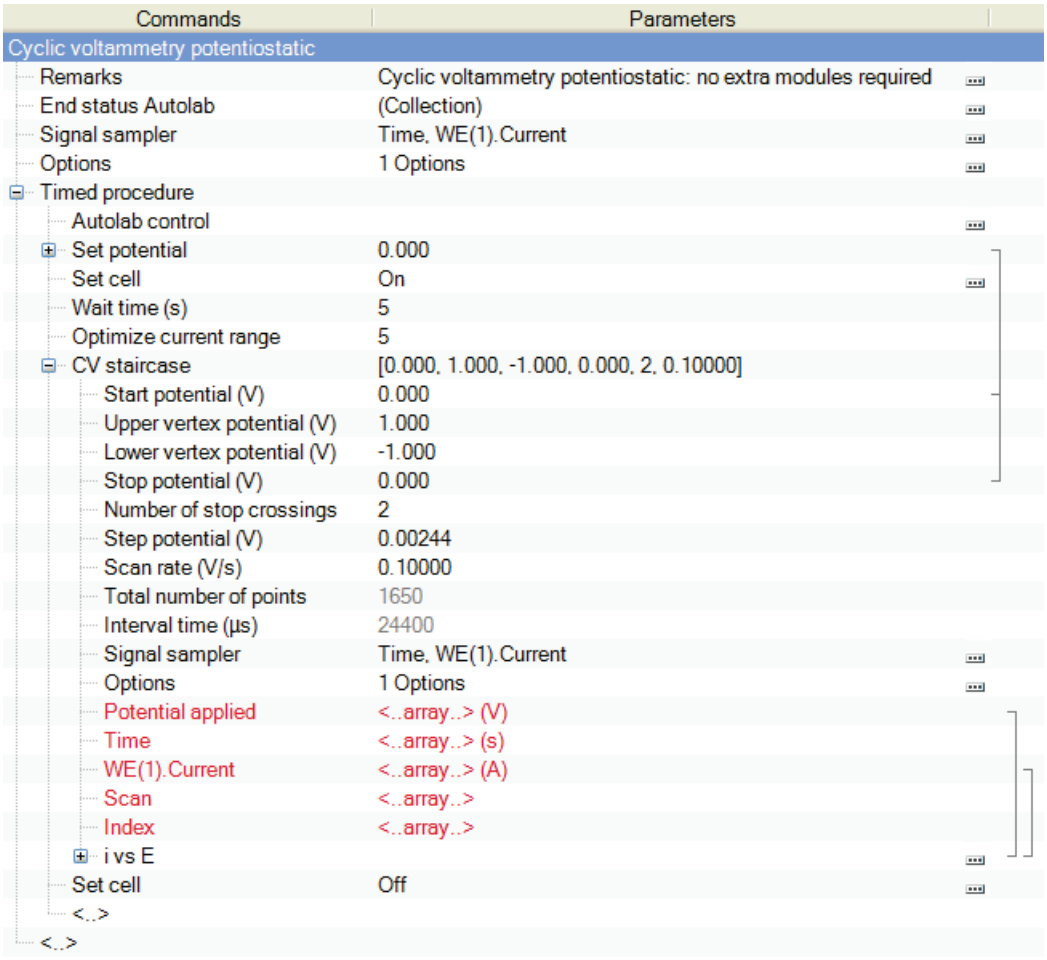


Figure 161 – The factory default Cyclic voltammetry potentiostatic procedure

New Autolab procedures

The following new factory default procedures have been added to the Autolab group (see Figure 162):

- Cyclic voltammetry with EQCM
- Cyclic voltammetry with BA
- Cyclic voltammetry with ECD
- Chrono potentiometry
- FRA impedance galvanostatic

Note: some of the Autolab factory default procedures have been renamed.

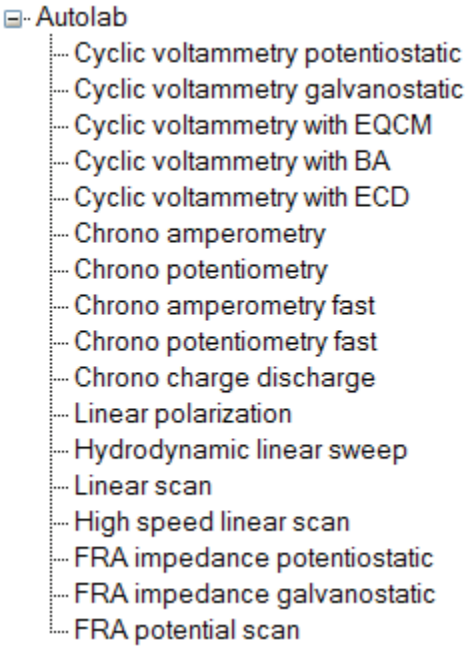


Figure 162 – The Autolab factory default procedures

Grouped commands

All the commands are now grouped in dedicated sections in the commands browser. Additional sections have been added, like the analysis sections, in which specific analysis commands can be found and the plot sections, in which ready made plot commands are located (see Figure 163).

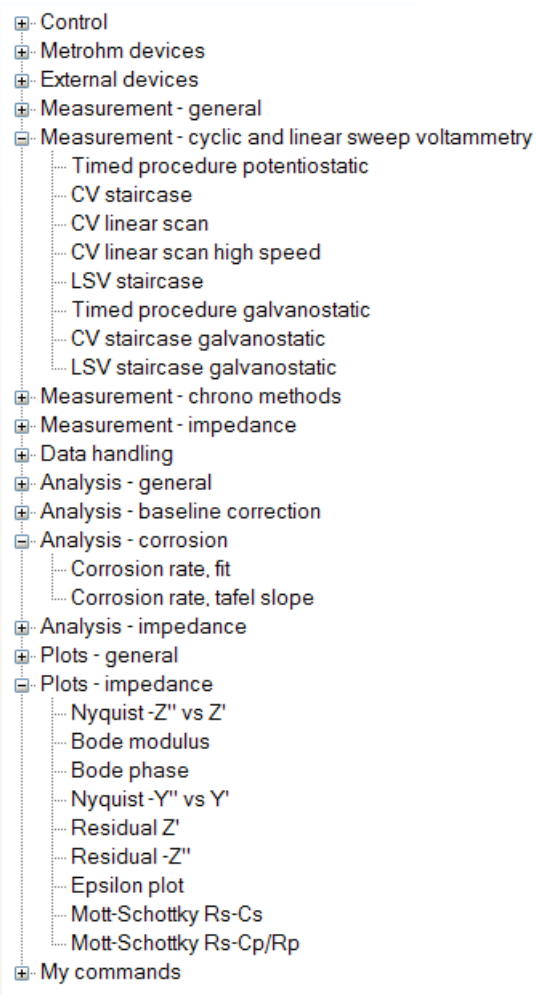


Figure 163 – The new commands browser, showing the details of the Cyclic and linear sweep voltammetry measurement section, the Corrosion analysis section and the Impedance plots section

Procedure templates

A series of special commands, called template commands, have been added to the command browser, in the Measurement – cyclic and linear sweep voltammetry and in the Measurement – chrono methods group (see Figure 164):

- Timed procedure potentiostatic
- Timed procedure galvanostatic

These commands are complete templates that can be used to construct procedures quickly.

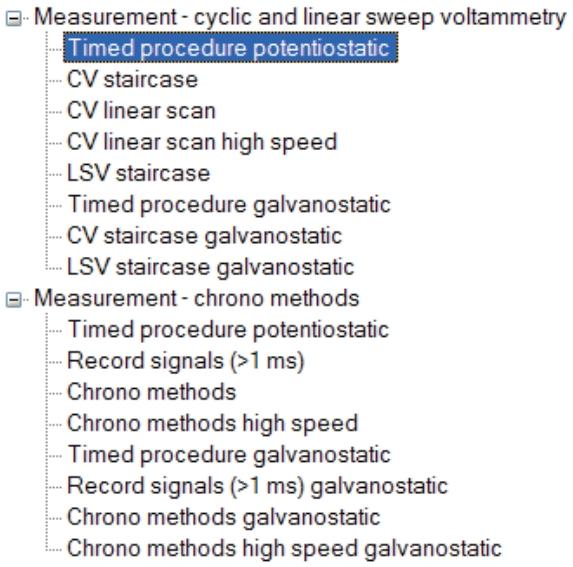


Figure 164 – Special commands are located in the Measurement – cyclic and linear sweep voltammetry and Measurement – chrono methods groups

When one of these commands is added to the procedure editor, a complete set of commands will be created. These commands constitute a complete template for a potentiostatic or galvanostatic measurement (see Figure 165).

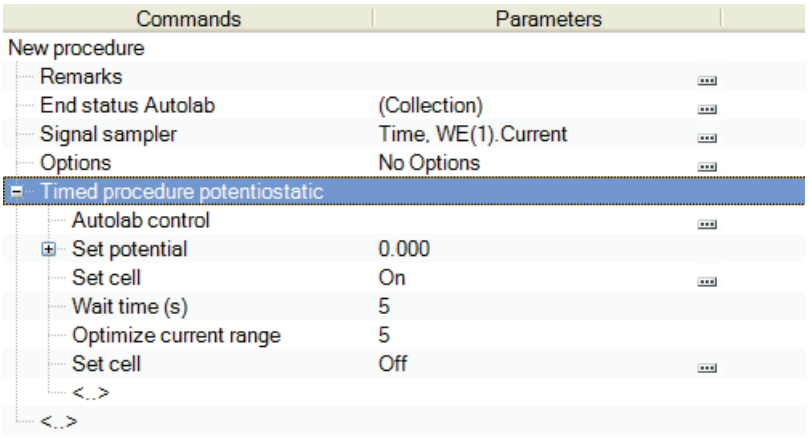


Figure 165 – The template commands can be used to create an almost complete procedure

Once a template command has been added to the procedure editor, the missing measurement command can be inserted in the template (see Figure 166). Additionally, the options and the sampler can be defined before the measurement is started. Start and stop potentials can be linked to the Set potential command, if required.

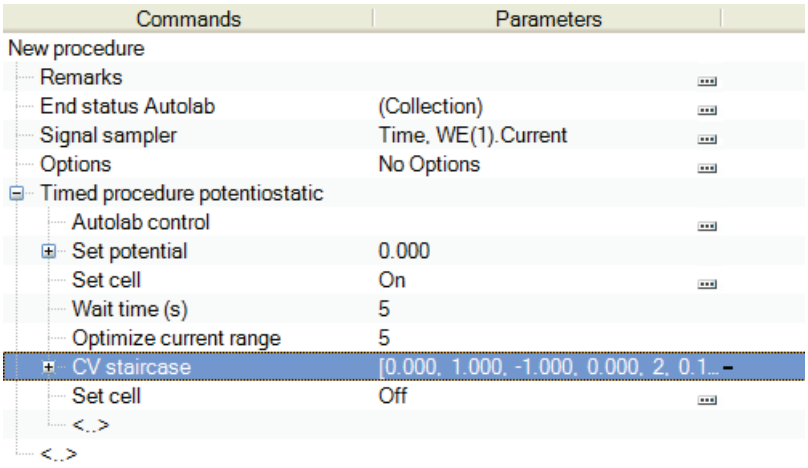


Figure 166 – Adding a measurement command to a template

New plotting framework

A new plotting framework has been implemented in this version of NOVA. It is now possible to add pre-defined plots to a procedure, by dragging and dropping the plot command onto a measurement command. If this measurement command provides the required pre-defined signals, these signals are automatically linked to the added plot.

The predefined plots are available in two different sections in the command browser. The Plots – general section contains pre-defined plots used in typical DC measurements. The Plots – impedance section contains pre-defined plots related to electrochemical impedance spectroscopy measurements (see Figure 167).

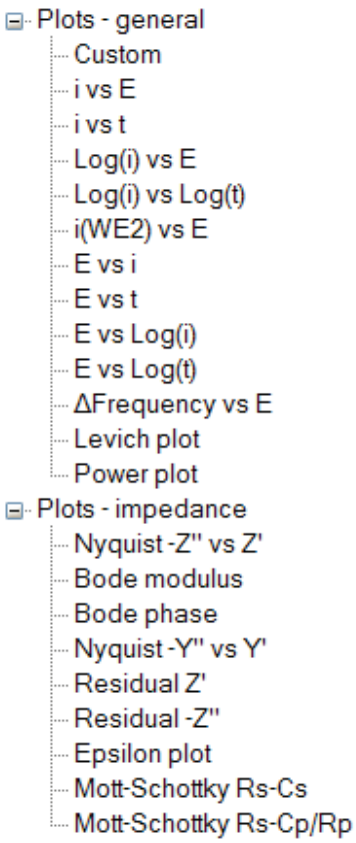


Figure 167 – The pre-defined default plots

The pre-defined plots are also available in the analysis view. Depending on the type of measurement, a number of predefined plots are available using the right-click menu in the analysis view. Figure 168 illustrates this feature on an impedance data set. Since the data has been recorded using the FRA frequency scan command, NOVA offers a number of impedance related plots.

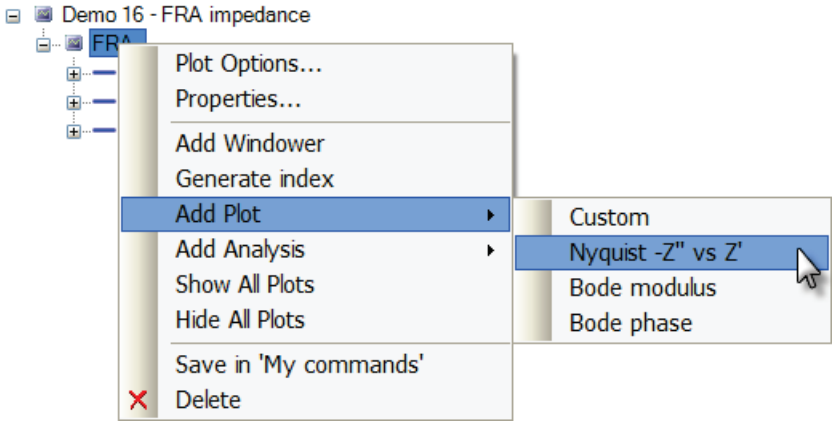


Figure 168 – Adding a pre-defined plot to a data set

The Custom plot is an empty plot, with undefined X, Y and Z signals. It is possible to add it using the list provided by the Add Plot menu or by clicking the Add Plot option in the right-click menu. The name of the plot can be changed using the right click-menu – properties option.

Note: Signal set, which was used in the previous versions of NOVA as name for a plot, has been renamed to Plot.

Previous NOVA versions and NOVA 1.4

It is possible to install both packages of the NOVA software on the same computer. Installing version 1.4 does not upgrade previously installed versions. However, it is not possible to use both software packages at the same time and data sets obtained with NOVA 1.4 cannot be used with previous versions of NOVA. The opposite situation is possible, using the conversion tools that are installed together with version 1.4.

DAC control in Autolab control

For external devices controlled through a DAC voltage (set using the Control external device command), a set DAC control field has been added to the Autolab control interface (see Figure 169). This allows for direct control of the DAC in a chrono methods (required for fast transient acquisition involving an external device) and for DAC control in the End Status Autolab (which is useful for safety reasons).

Note: only DAC channel #3 can be used using this control.

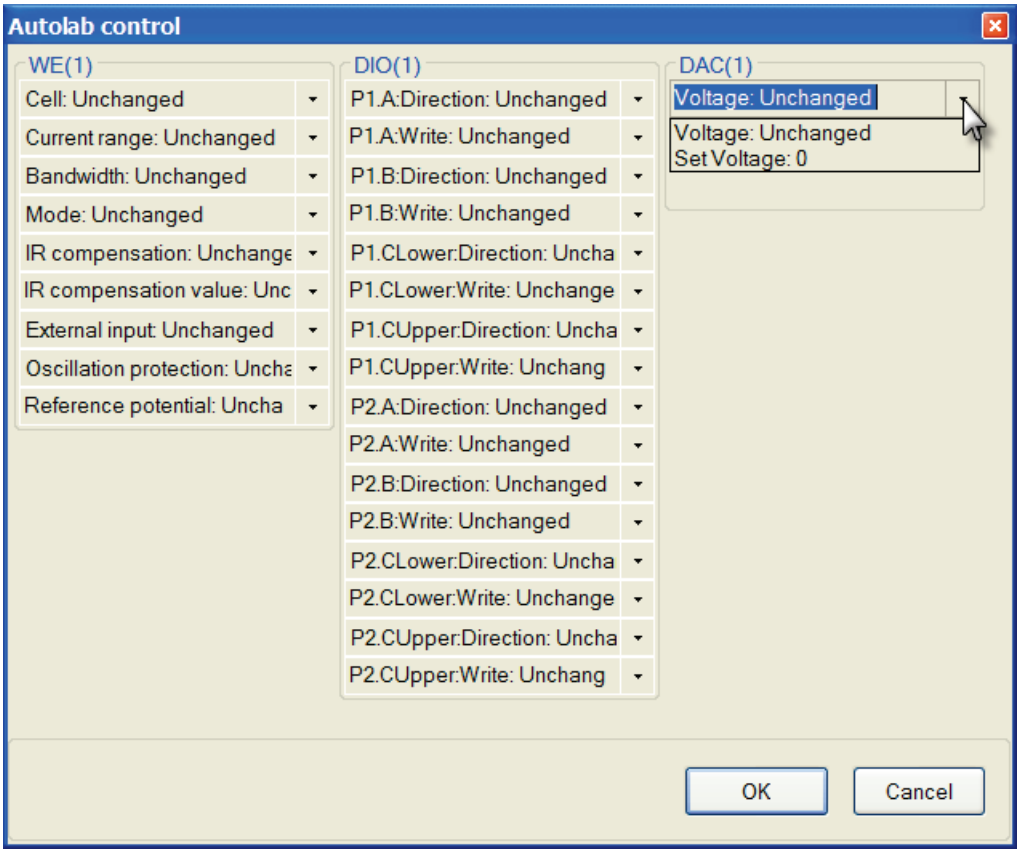


Figure 169 – DAC control in the Autolab control window

Cutoffs

The options available in NOVA have been augmented with a Cutoff interface. It is now possible to define any cutoff condition in a procedure. The cutoff conditions can be defined for the whole procedure or a specific measurement command. It is possible to group cutoff conditions using OR and AND operators. Moreover, users can define the number of cutoff conditions detections required to trigger the cutoff actions. Finally, when a cutoff condition is met, the user has the choice to stop the command, stop the timed procedure or stop the whole procedure (see Figure 170).

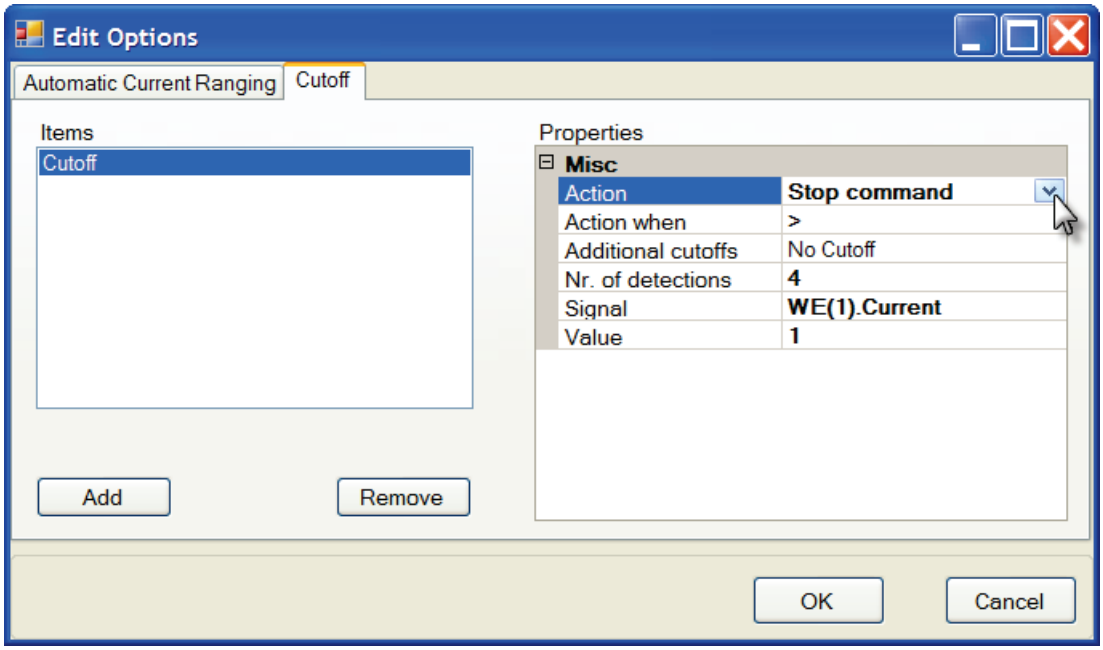


Figure 170 – The Cutoff interface

More information about the cutoffs can be found in the Cutoff tutorial.

Simplified FRA frequency range editor

The determine FRA range window has been simplified. The amplitude range builder has been removed. The possibility of defining more than one amplitude is still available, using the Add button. Moreover, it is now possible to define the amplitude of the FRA frequency scan in absolute value (top) or root mean square value (rms). The tooltip displays both values (see Figure 171).

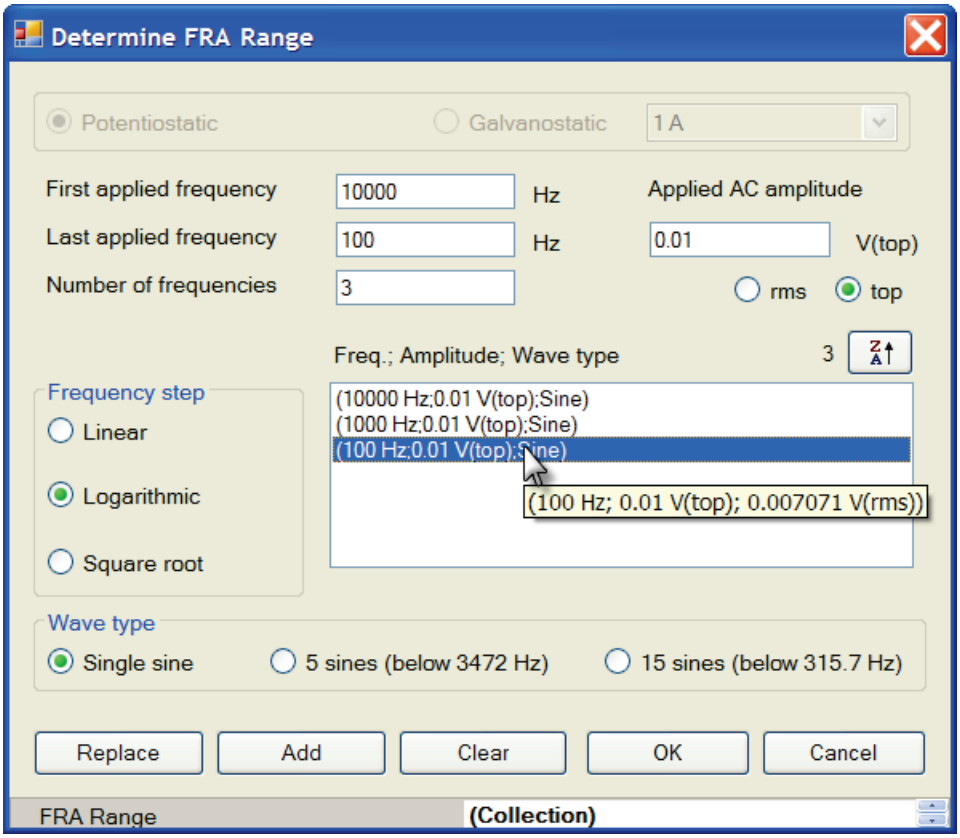


Figure 171 – The simplified determine FRA range window

FRA Galvanostatic support

A dedicated FRA measurement galvanostatic command has been added to the command list. This command can be used to define a frequency scan in galvanostatic conditions. The amplitude can be defined in A directly (see Figure 172).

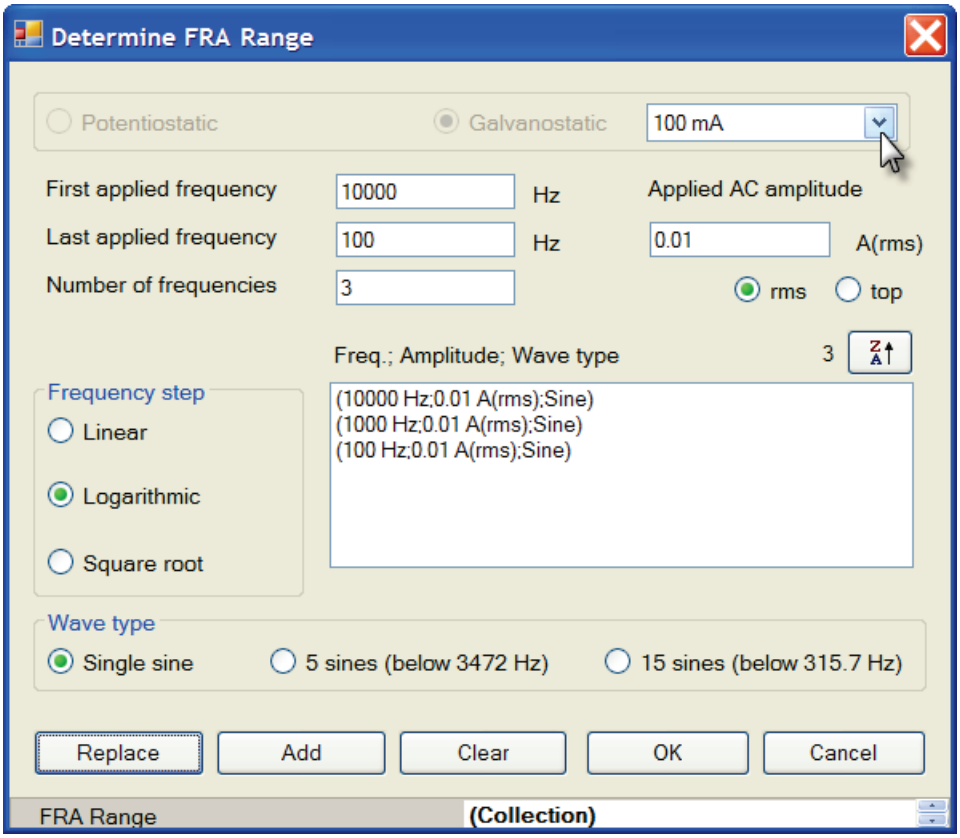


Figure 172 – The GSTAT FRA range builder window

NOTE: Automatic current ranging is not possible in GSTAT mode.

Reverse compatibility with previous NOVA versions

This version of NOVA introduces a large number of changes that affect the way the software reads and writes data files. In order to ensure backwards compatibility with the previous versions, conversion tools are provided.

The conversion tool can be used to convert data recorded with previous versions. The conversion process is summarized Figure 173. Data from NOVA 1.2 is stored in a single *.yap* file, which is first converted to files in the NOVA 1.3 format[13]. Data from NOVA 1.3 is available as single *.nox* files can be converted into NOVA 1.4 *.nox* files.

[13] More information can be found in the NOVA 1.3 release notes.

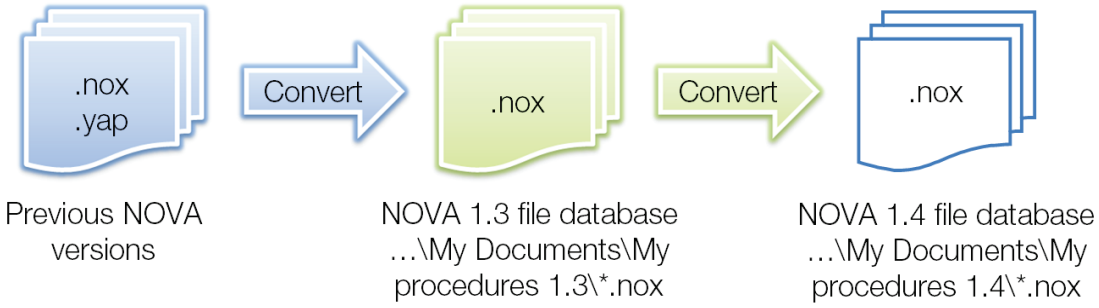


Figure 173 – Schematic view of the conversion process to NOVA 1.4 from previous versions

After installing NOVA 1.4, start the *Upgrade files to NOVA 1.4* application (Start menu – All Programs – Autolab – Tools).

The Upgrade to NOVA application will be started (see Figure 174). To use the upgrade function, files from older NOVA version must be added to the application, as individual *.nox* files.

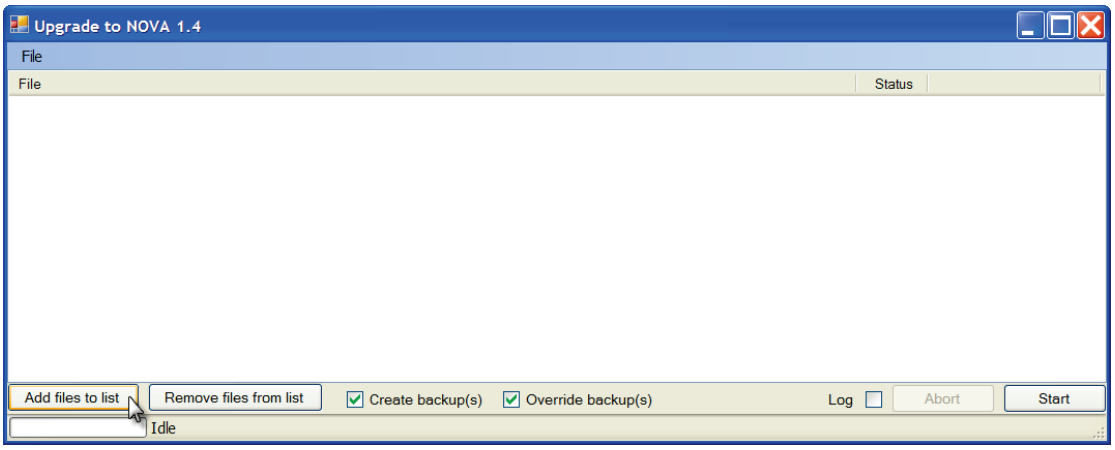


Figure 174 – The Upgrade to NOVA 1.4 application

To add files to the list, press the 'Add files to list' button. Navigate to the folder containing the files to upgrade from previous NOVA versions to 1.4 (see Figure 175).

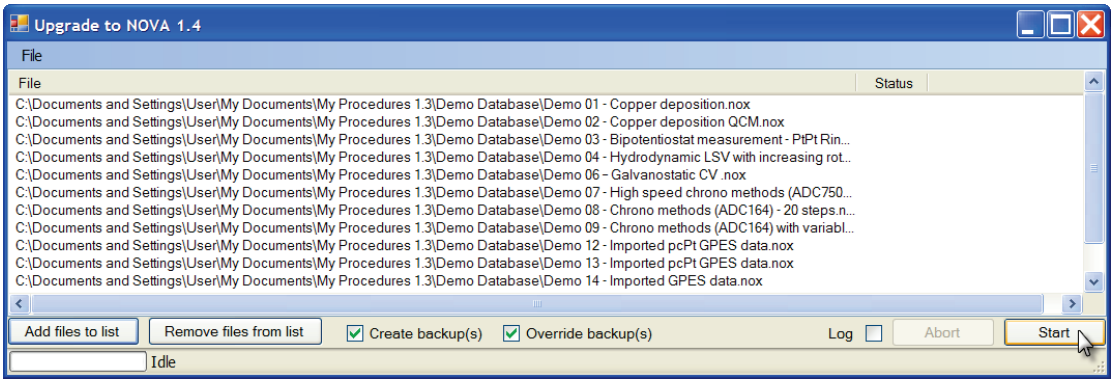

Upgrade to NOVA 1.4
File
File
Status
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 01 - Copper deposition.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 02 - Copper deposition QCM.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 03 - Bipotentiostat measurement - PtPt Rin...
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 04 - Hydrodynamic LSV with increasing rot...
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 06 - Galvanostatic CV .nox
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 07 - High speed chrono methods (ADC750...
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 08 - Chrono methods (ADC164) - 20 steps.n...
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 09 - Chrono methods (ADC164) with variabl...
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 12 - Imported pcPt GPES data.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 13 - Imported pcPt GPES data.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 14 - Imported GPES data.nox
Add files to list
Remove files from list
Create backup(s)
Override backup(s)
Log
Abort
Start
Idle

Figure 175 – Adding the files to the list

Note: the original files will not be removed, which means that you can still access the data from previous NOVA versions.

Click the Start button to initiate the conversion to the NOVA 1.4 file format. It is possible to create a backup of the source files and to overwrite the backup files if they are already found in the source folder. It is also possible to create a log file, which can be useful if the conversion fails.

During the upgrade step, the progress is displayed in real time (see Figure 176).

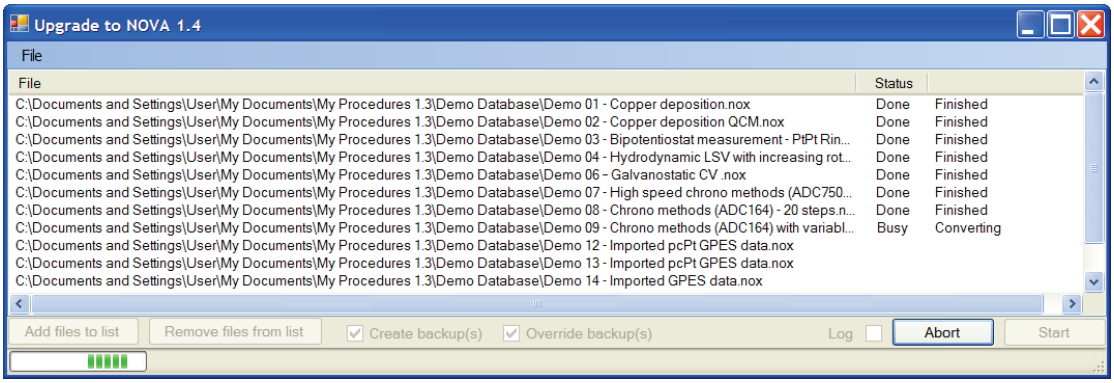

Upgrade to NOVA 1.4
File
File
Status
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 01 - Copper deposition.nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 02 - Copper deposition QCM.nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 03 - Bipotentiostat measurement - PtPt Rin... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 04 - Hydrodynamic LSV with increasing rot... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 06 - Galvanostatic CV .nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 07 - High speed chrono methods (ADC750... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 08 - Chrono methods (ADC164) - 20 steps.n... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 09 - Chrono methods (ADC164) with variabl... Busy Converting
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 12 - Imported pcPt GPES data.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 13 - Imported pcPt GPES data.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 14 - Imported GPES data.nox
Add files to list
Remove files from list
Create backup(s)
Override backup(s)
Log
Abort
Start

Figure 176 – The upgrade application converts every *.nox* file in the list from to the NOVA 1.4 format

When all the .nox files have been processed, they will be compatible with the NOVA 1.4 format (see Figure 177).

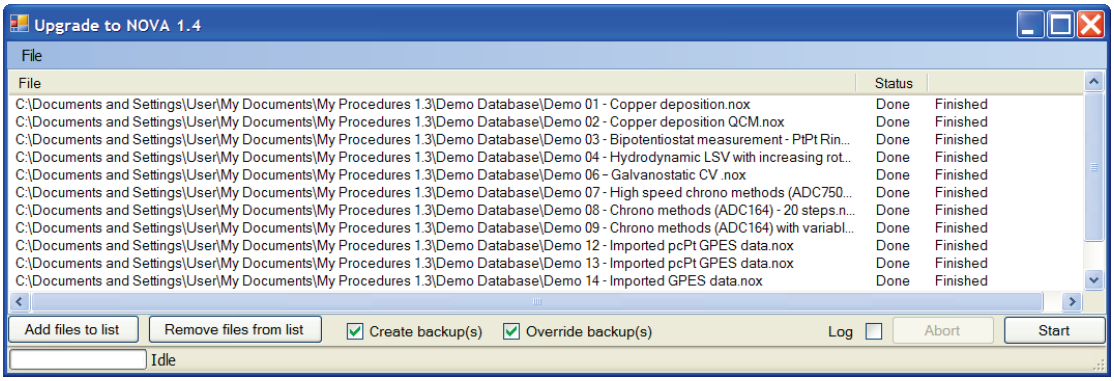

Upgrade to NOVA 1.4
File
File
Status
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 01 - Copper deposition.nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 02 - Copper deposition QCM.nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 03 - Bipotentiostat measurement - PtPt Rin... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 04 - Hydrodynamic LSV with increasing rot... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 06 - Galvanostatic CV .nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 07 - High speed chrono methods (ADC750... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 08 - Chrono methods (ADC164) - 20 steps.n... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 09 - Chrono methods (ADC164) with variabl... Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 12 - Imported pcPt GPES data.nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 13 - Imported pcPt GPES data.nox Done Finished
C:\Documents and Settings\User\My Documents\My Procedures 1.3\Demo Database\Demo 14 - Imported GPES data.nox Done Finished
Add files to list
Remove files from list
Create backup(s)
Override backup(s)
Log
Abort
Start
Idle

Figure 177 – When the upgrade application has finished, the converted *.nox* files will be ready for NOVA 1.4

Note: if the location of the NOVA source database is the My Documents\My Procedures 1.x folder, the converted files will be automatically copied to the My Documents\My Procedures 1.4 folder. If the source database is located in another folder, the same folder will be used as location for the NOVA 1.4 *.nox* files.

New data analysis framework and data analysis tools

The data analysis framework has been redesigned. It is now possible to add data analysis tools directly to the data in the Analysis view, by using a context menu. By right-clicking on a plot in NOVA in the data explorer frame it is possible to add analysis tools directly to the plot (see Figure 178).

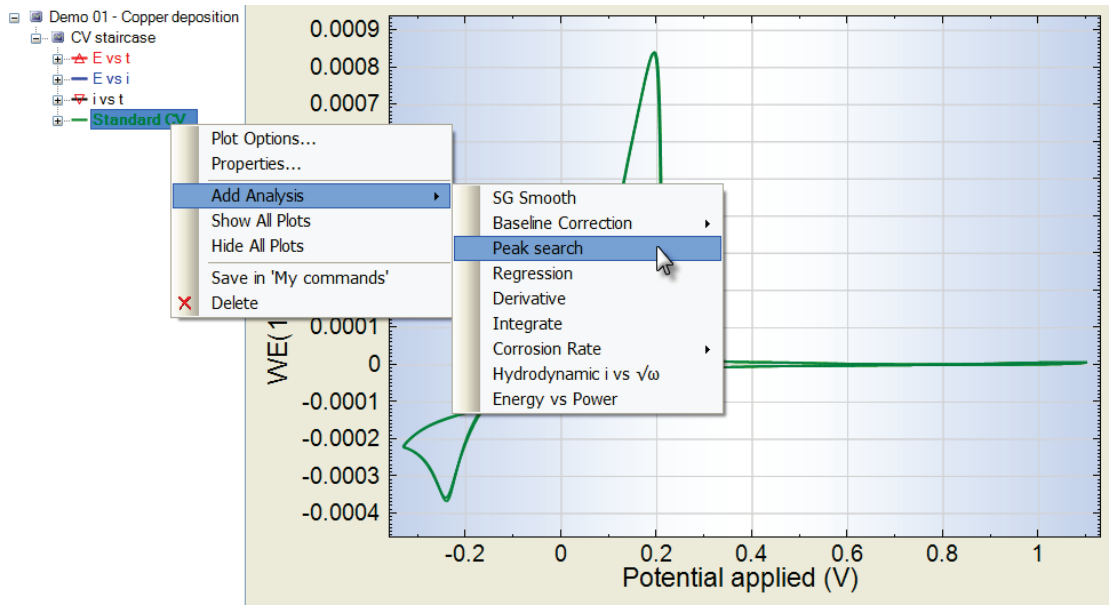


Figure 178 – Adding a peak search to a CV staircase plot ½

Analysis tools added to a plot are displayed directly in the data explorer frame and the control parameters of the selected tool are accessed using a dedicated interface in the Analysis frame (see Figure 179).

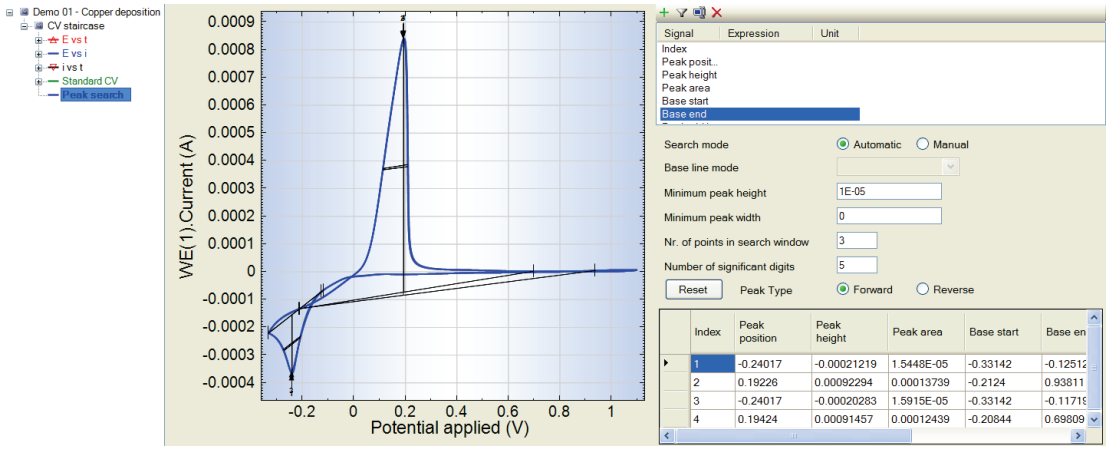


Figure 179 – Adding a peak search analysis tool to a CV staircase 2/2

The results of the data analysis tools are available in the data grid. This allows for easy export of the results to an ASCII or .xls file (see Figure 180).

	Index	Peak position	Peak height	Peak area	Base start	Base end	Peak width half	Peak (1/2)	Peak sum of derivatives
▸	1	-0.24017	-0.00021219	1.5448E-05	-0.33142	-0.12512	0.06295	-0.031234	0.0085256
	2	0.19226	0.00092294	0.00013739	-0.2124	0.93811	0.096703	0.080468	0.1029
	3	-0.24017	-0.00020283	1.5915E-05	-0.33142	-0.11719	0.069135	-0.0342	0.0073167
	4	0.19424	0.00091457	0.00012439	-0.20844	0.69809	0.097145	0.080772	0.10011

Figure 180 – Data analysis results are available in the data grid

Furthermore, the results of the data analysis tools can be used to generate new plots (see Figure 181). It is also possible to use the *Calculate signals* and *Filter and select* tools directly, without switching to the Data grid.

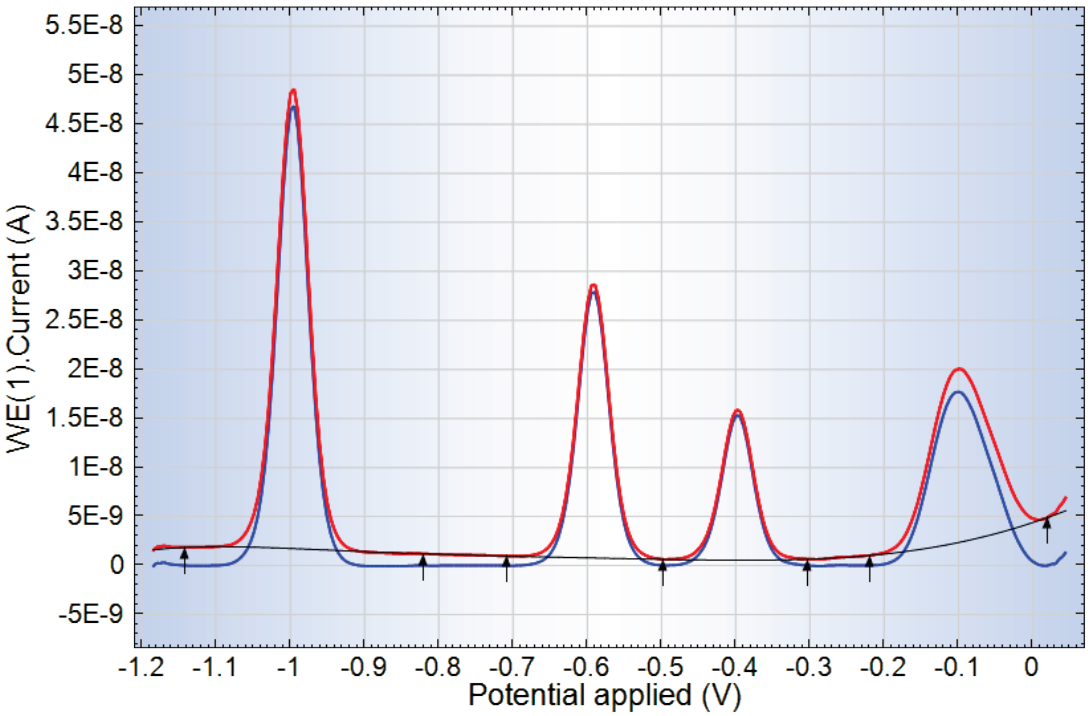


Figure 181 – Stacked plots and data analysis tools: the red line is the original plot, the black line the applied baseline correction and the blue line is the corrected plot

New data handling and analysis commands

NOVA 1.4 introduces a number of new data analysis commands, which can be used to perform automatic data handling and data analysis.

The following commands have been added:

- In the Data handling group
  - Import ASCII
  - Export ASCII
  - Scan extractor
- In the Analysis – general group
  - Regression
  - Integrate
  - Calculate charge
  - Energy vs Power
  - Hydrodynamic i vs $\sqrt{\omega}$
- In the Analysis – baseline correction group
  - Polynomial fixed order
  - Polynomial maximum order
  - Exponential
  - Circle
- In the Analysis – corrosion group
  - Corrosion rate, fit
  - Corrosion rate, Tafel slope
- In the Analysis – impedance group

- Kronig-Kramers test
- Include all FRA data

Furthermore, the following commands have been renamed:

- Automatic peak search → Peak search
- Mathematical parser → Calculate signal
- Signal windower → Windower

My commands

It is now possible to define your own commands using the My commands framework. In Nova 1.4, a new database that be used to store your own commands has been added. This database can be defined using the database manager (see Figure 182).

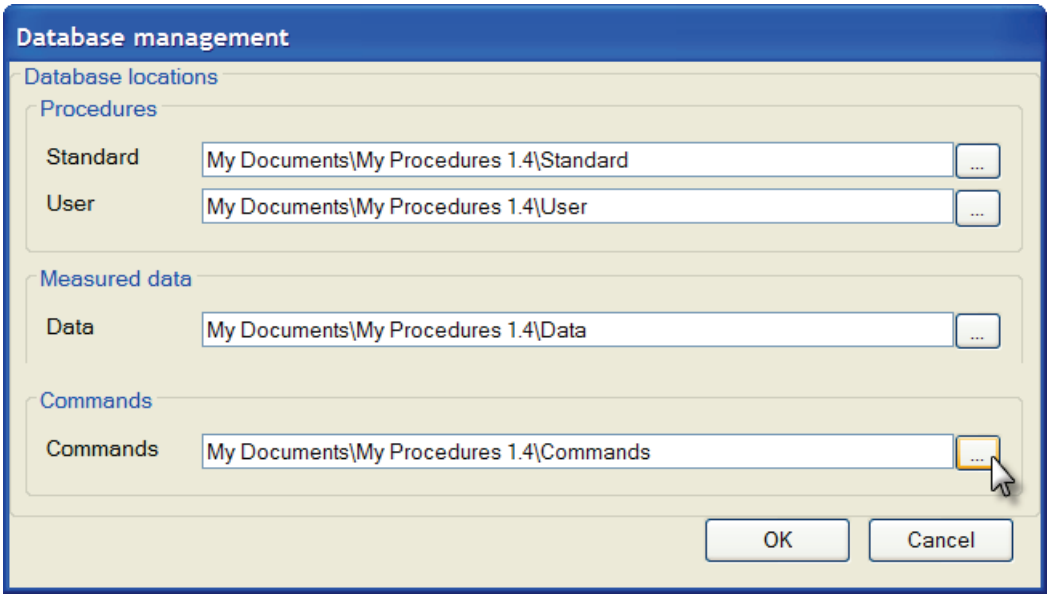


Figure 182 – The database manager can be used to define a Commands database

Commands defined using the My commands framework will be stored in the defined database and will be available for procedure building in the commands browser (see Figure 183).

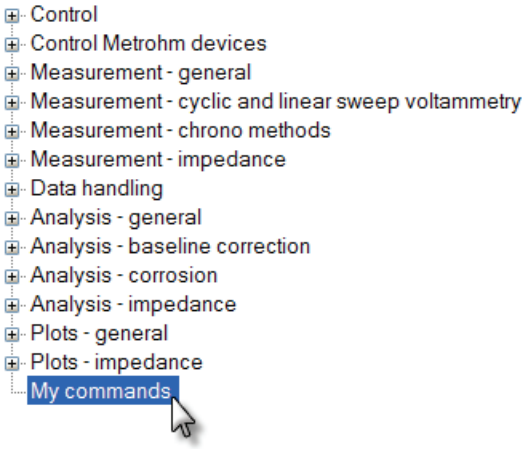


Figure 183 – The My commands group is located in the commands browser

To add a command to the My commands database, right-click the command in the procedure editor and select the 'Save in My commands' option (see Figure 184).

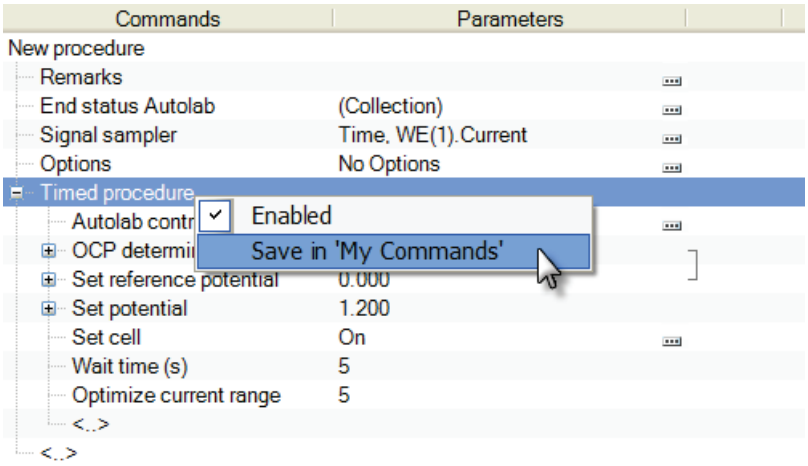


Figure 184 – Click the Save in My Commands option to add it to the My commands database

You will be prompted to specify a name for the command (see Figure 185).

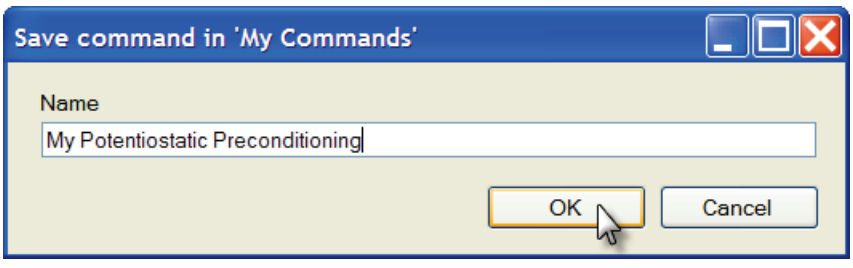


Figure 185 – Specify a name for the command

In the example shown here, the whole Timed procedure will be saved in the My commands database, as My potentiostatic Preconditioning (see Figure 186).

Note: a tooltip displays the details of the command.

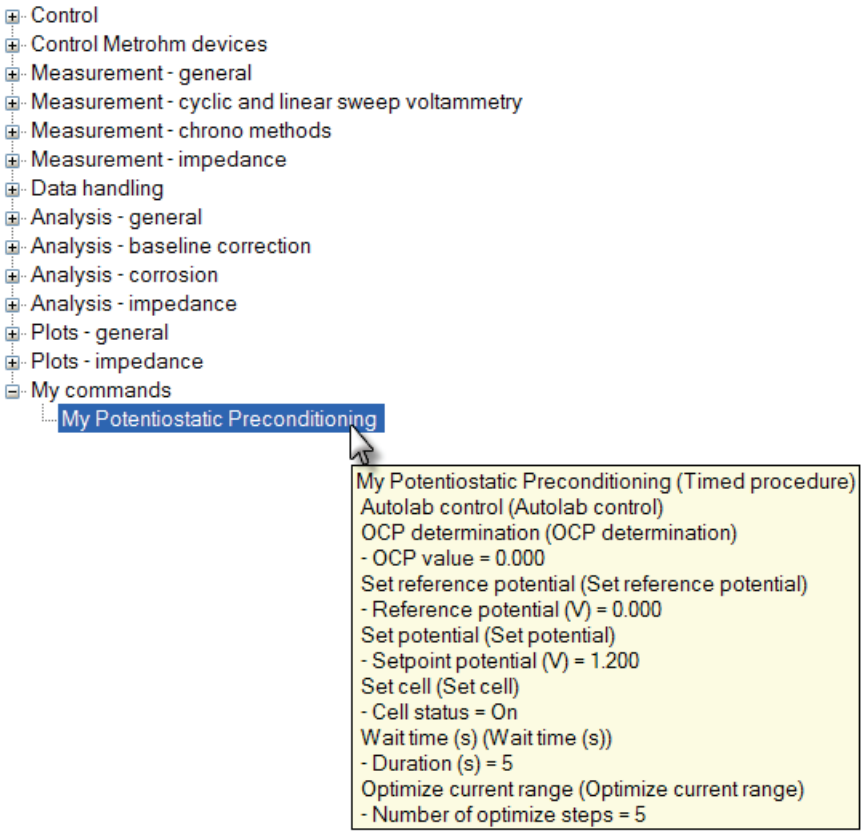

Control
Control Metrohm devices
Measurement - general
Measurement - cyclic and linear sweep voltammetry
Measurement - chrono methods
Measurement - impedance
Data handling
Analysis - general
Analysis - baseline correction
Analysis - corrosion
Analysis - impedance
Plots - general
Plots - impedance
My commands
My Potentiostatic Preconditioning
My Potentiostatic Preconditioning (Timed procedure)
Autolab control (Autolab control)
OCP determination (OCP determination)
- OCP value = 0.000
Set reference potential (Set reference potential)
- Reference potential (V) = 0.000
Set potential (Set potential)
- Setpoint potential (V) = 1.200
Set cell (Set cell)
- Cell status = On
Wait time (s) (Wait time (s))
- Duration (s) = 5
Optimize current range (Optimize current range)
- Number of optimize steps = 5

Figure 186 – The command is added to the My commands database

Once a command has been added to the My command database, it can dragged into the procedure editor as any other command. In the example shown in Figure 187, the My Potentiostatic Preconditioning command has been added to a new procedure.

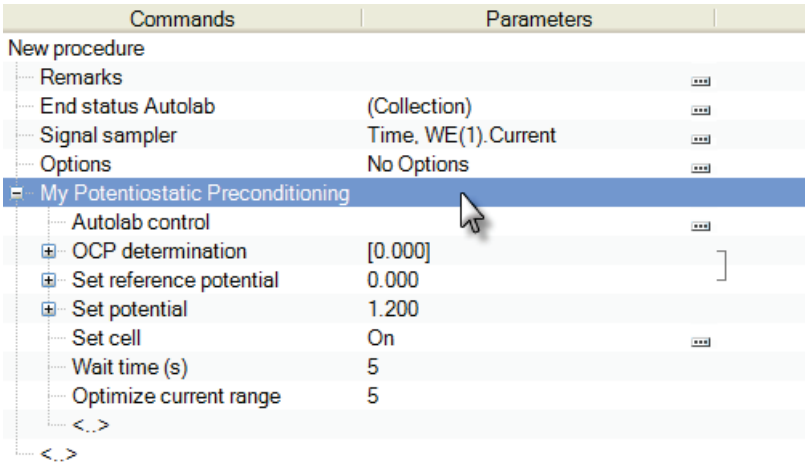


Figure 187 – Adding a My command into the procedure editor creates a copy of the original command

Note: saving a complete Timed procedure instead of a single command allows you to very quickly group commands. This simplifies the procedure building process, especially for routine measurements.

Improved Import GPES command

The import GPES command has been improved. It is now possible to define the number of columns in the GPES data file (see Figure 188). This allows you to import GPES data files with a recorded second signal (bipotentiostat, SPR, etc…).

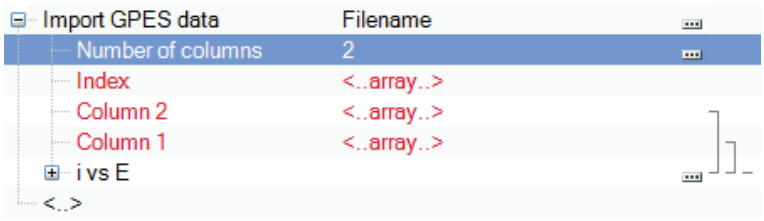


Figure 188 – The Import GPES data command

Moreover, it is possible to assign names and units to the columns located in the GPES file, using a dedicated interface (accessible by clicking the … located on the Number of columns parameter line). Using the Signal editor window, it is possible to change the name of the columns manually or using a drop-down list (see Figure 189).

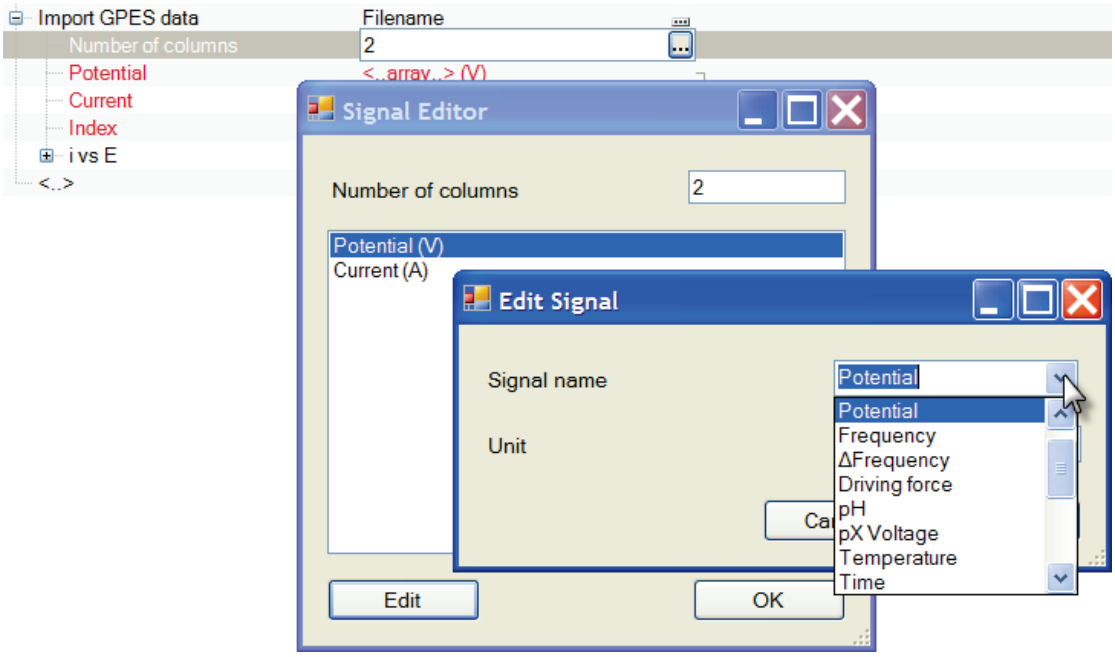


Figure 189 – Changing the name of the columns can be done using the Signal Editor window

Note: using the names from the drop-down list allows identifying the signals and ensures compatibility with all the data analysis tools.

Import and Export ASCII

Import and Export ASCII data commands have been added to the data handling command group. These two commands can be used to import data from an ASCII file or export measured electrochemical signals to an ASCII file.

The Import ASCII data has a number of parameters like the number of lines to ignore at the beginning of the file, the number of columns in the file, the column delimiter (see Figure 190).

Figure 190 – The import ASCII data command

Moreover, it is possible to specify the name of the signals using the same interface as the new Import GPES command.

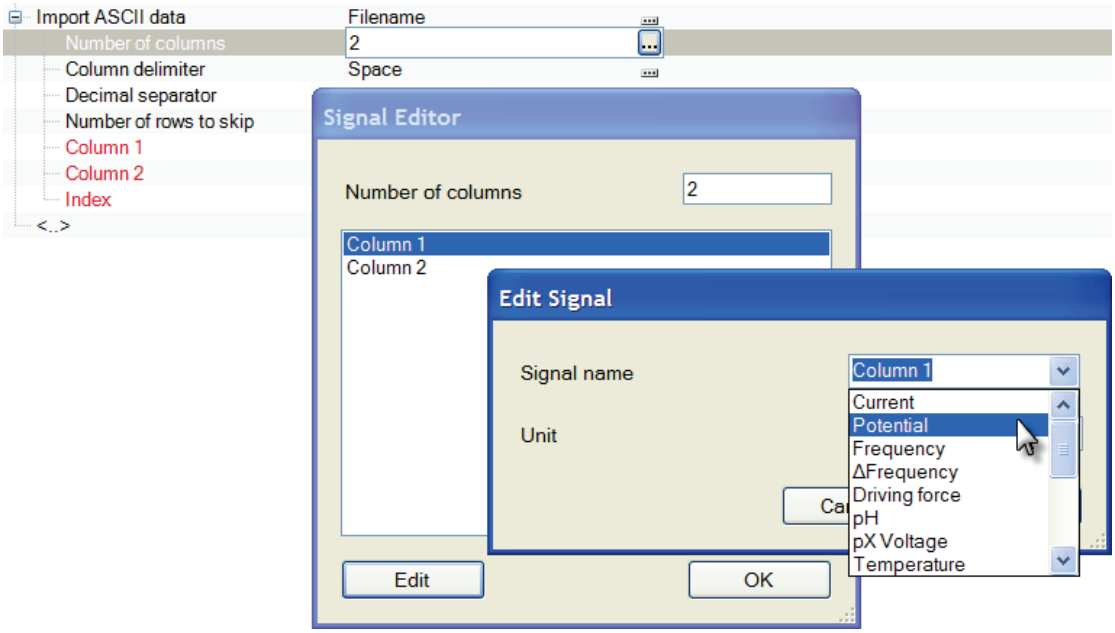


Figure 191 – Changing the name of the columns can be done using the Signal Editor window

The Export ASCII data command can be used to export measured or calculated electrochemical signals during a measurement. The number of columns and the delimiter can be specified, as well as the filename (see Figure 192).

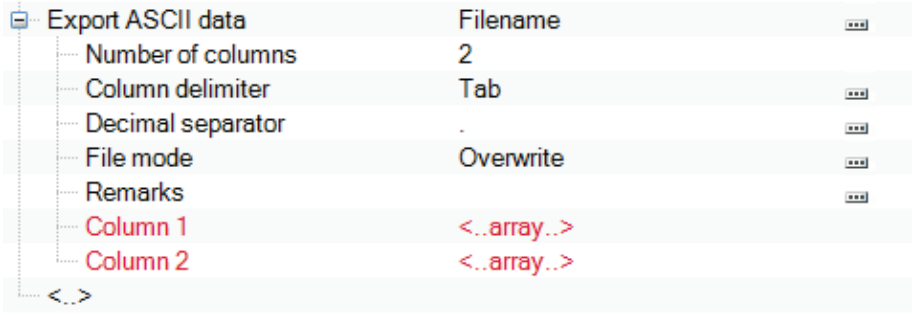


Figure 192 – The export ASCII data command

The Columns can be linked to the electrochemical signals to export (see Figure 193).

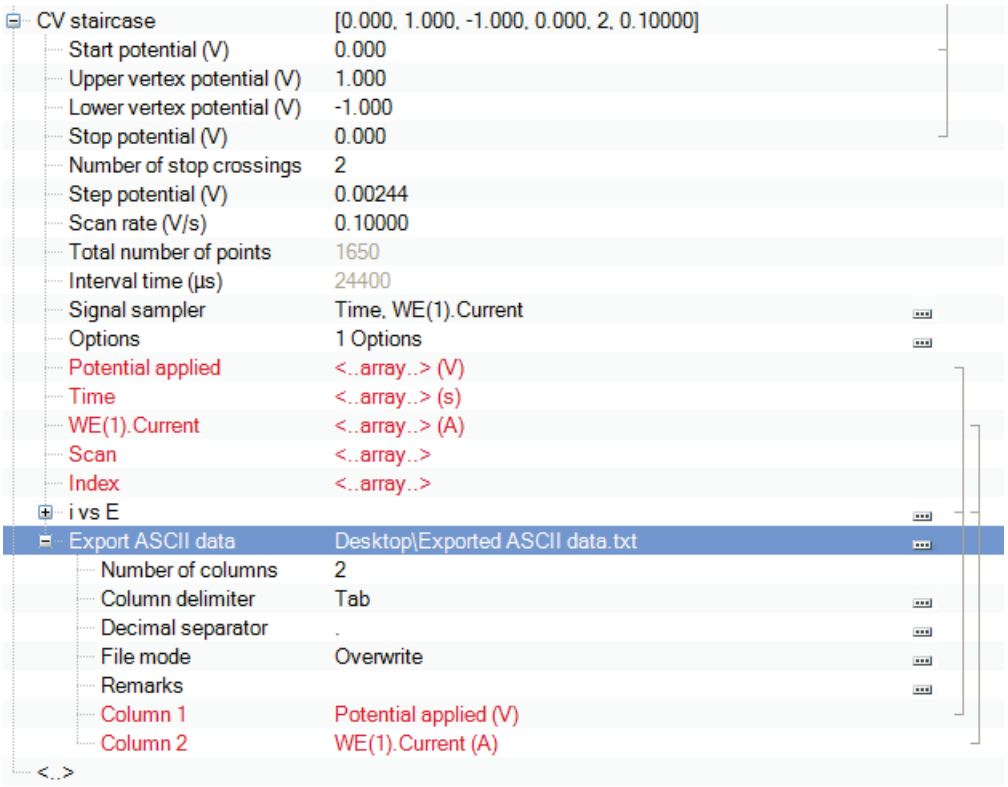


Figure 193 – Using the Export ASCII data in combination with a CV staircase command

Note: exporting data to an ASCII file during a measurement introduces a delay in the timing. The duration of the pause depends on the amount of data points.

G circuit element

The Gerischer diffusion circuit element, which is used to model the effect of a preceding chemical reaction happening in the bulk solution (so-called CE mechanism) or the behavior of a porous electrode, has been added to the list of available circuit elements in the Fit and Simulation tool (see Figure 194).

- G, Gerischer impedance $$Z_G = \frac{1}{Y_0\sqrt{(k_a + j\omega)}}$$

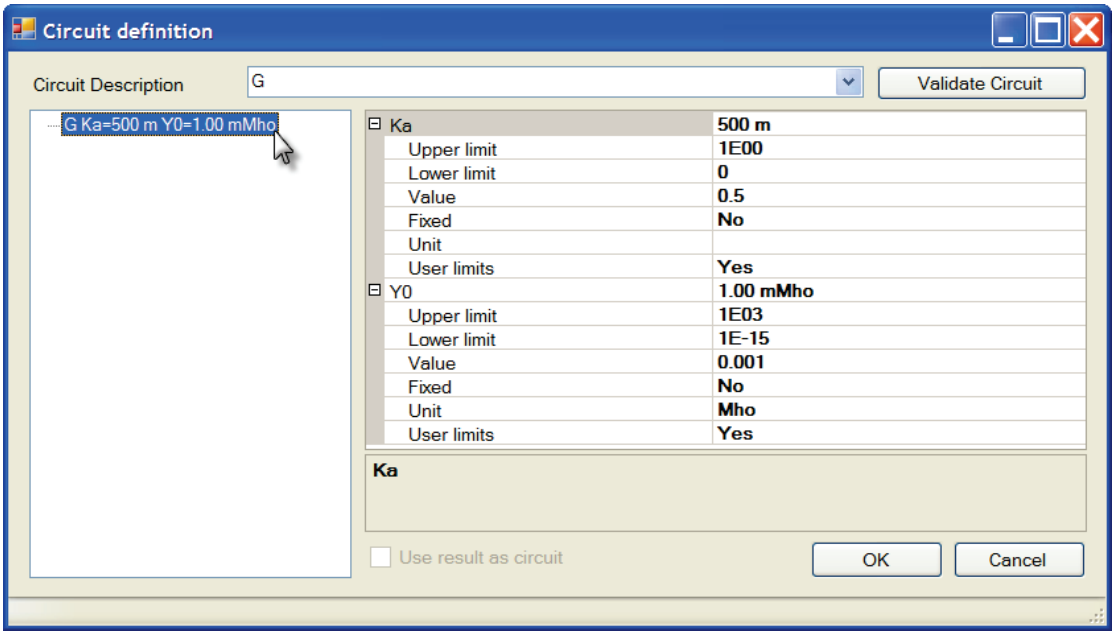


Figure 194 – The G element is now available in the Fit and Simulation

Kronig-Kramers calculation

The Kronig-Kramers (KK) test tool has been added to the current version of NOVA. The KK test is often used to relate the real and imaginary parts of a complex transfer function (like electrochemical impedance, Z). This test can be used to check whether the measured data comply with the assumptions of KK transformation. These assumptions are:

1. The response is only related to the excitation signal.
2. The response is linear (or the perturbation is small, e.g. <10 mV, for non-linear systems).
3. The system does not change with time.
4. The system is finite for all values of ω, including zero and infinity.

If the investigated system changes with time due to e.g. ageing, temperature change, non-equilibrium initial state etc., the test fails. Failure of KK test usually means that no good fit can be obtained using the equivalent circuit method. This analysis tool is based on the work of Dr. B.A. Boukamp as published in J. Electrochem. Soc., Vol 142, 6 (1995).

The KK test can be used by using the right-click menu and by choosing Kronig-Kramers test from the Add Analysis menu (see Figure 195).

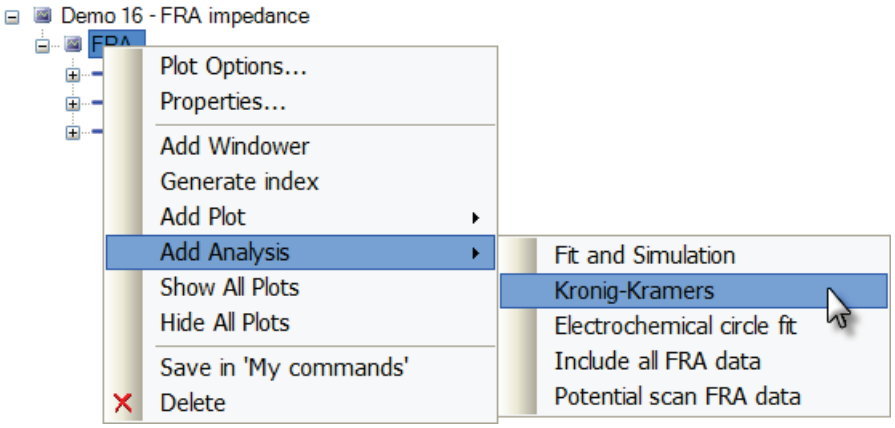


Figure 195 – Adding the Kronig-Kramers test to impedance data

Note: in the current version of NOVA, only the impedance Kronig-Kramers test, which uses a serial (RC) element sequence, is supported.

More information about the Kronig-Kramers test can be found in the Impedance measurements tutorial.

Metrohm devices support

This version of NOVA introduces the support for the Metrohm 800 Dosino, Metrohm 801 Stirrer and Metrohm 814/815/858 Sample changer through the Metrohm Serial Bus (MSB) interface. A Control Metrohm devices command group is available in the commands browser (see Figure 196).

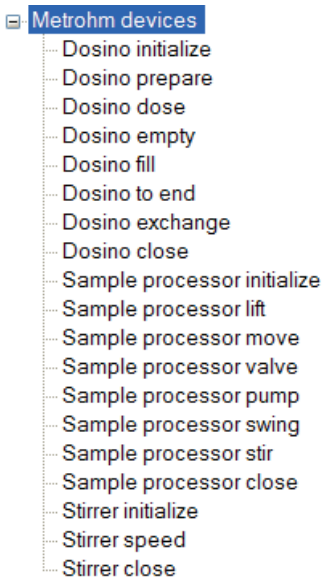


Figure 196 – The Dosino related commands are located in the Control Metrohm devices group

More information about the Dosino control can be found in the External devices tutorial.

External devices support

This version of NOVA also supports the RS232 communication protocol, which can be used to control external devices, like water baths, stirrers, valves, etc…

The External devices commands are located in the External devices group (see Figure 197).

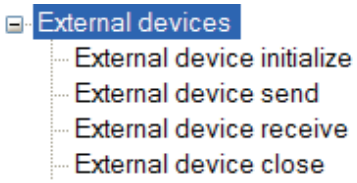


Figure 197 – The External devices commands can be used to setup a RS232 communication protocol

More information about the External devices control can be found in the External devices tutorial.

NOVA 1.3 Release notes (Released 01/04/2008)

Introduction

These notes provide an overview of the new features introduced in NOVA 1.3 compared to the previous release.

The following items have been added to NOVA 1.3:

- A number of tutorials, available from the Help menu

- Support for the modules

  - Booster 10 A
  - Booster 20 A

- Support for the instruments

  - PGSTAT 100
  - PGSTAT 30/302(N)
  - PGSTAT 12

- Improvements and additions

  - NOVA 1.2 and NOVA 1.3 on the same computer
  - Improved Chrono methods
  - SCANGEN/SCAN250 together with the ADC164
  - New linking behavior
  - Printing links (procedure setup)
  - Reverse compatibility with version 1.2
  - Diagnostics
  - Signal set(s) for each measurement command
  - More than one signal set in the measurement view
  - Clear plot measurement
  - Manual scaling during measurement
  - Mathematical parser as a command
  - Improved Autolab Control interface
  - OCP integration
  - Reference voltage command
  - Import FRA data command
  - Find circle for impedance data
  - Fit and simulation for impedance data

Tutorials

A series of short tutorials is available from the Help menu in Nova. Each tutorial is dedicated to a specific measurement technique or aspect of the software.

Some tutorials include procedures that can be used to perform simple measurements on the Autolab dummy cell.

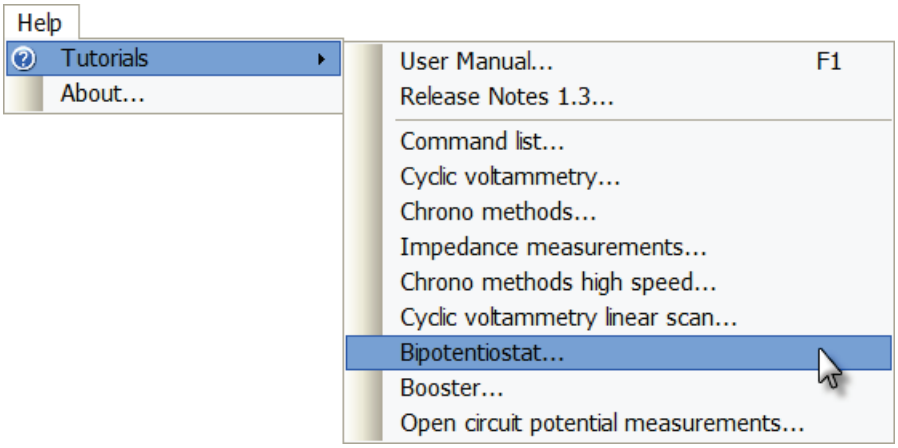


Figure 198 – A series of short tutorials is available from the Help menu

Modules support

NOVA 1.3 introduces the support for the current boosters (Booster 10A and Booster 20A). The boosters can be used by setting the instrument in the highest current range (10 A or 20 A).

Note: the boosters can only be used on DIO connector P1.

Hardware support

The hardware setup of NOVA 1.3 now includes the PGSTATs 12, 30, 302N and 100. The hardware setup now separates the choice of the main Autolab module and the additional modules (see Figure 160).

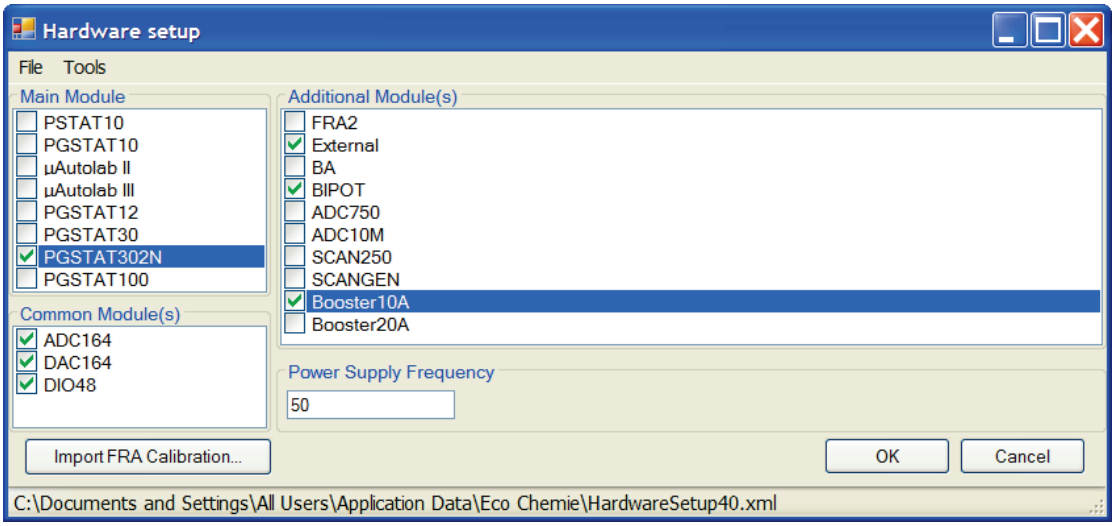


Figure 199 – The hardware setup window

NOVA 1.2 and NOVA 1.3

It is possible to install both packages of the NOVA software on the same computer. Installing version 1.3 does not upgrade version 1.2. However, it is not possible to use both software packages at the same time and data sets obtained with NOVA 1.3 cannot be used with version 1.2. The opposite situation is possible, using the conversion tools that are installed together with version 1.3 (see page 9).

Improved Chrono Methods

The Chrono methods command introduced in NOVA 1.2 had a USB timeout limitation which meant that measurements longer than 25 seconds could not be performed. This limitation was not practical for long measurements and it has been resolved in NOVA 1.3. Using the Chrono methods command, it is now possible to measure the response of the electrochemical cell as long as required. Figure 200 shows the potential profile for a Chrono methods measurement, with a total duration of 60 seconds (40 repetitions of a sequence of three potential steps – total number of points: 60.000).

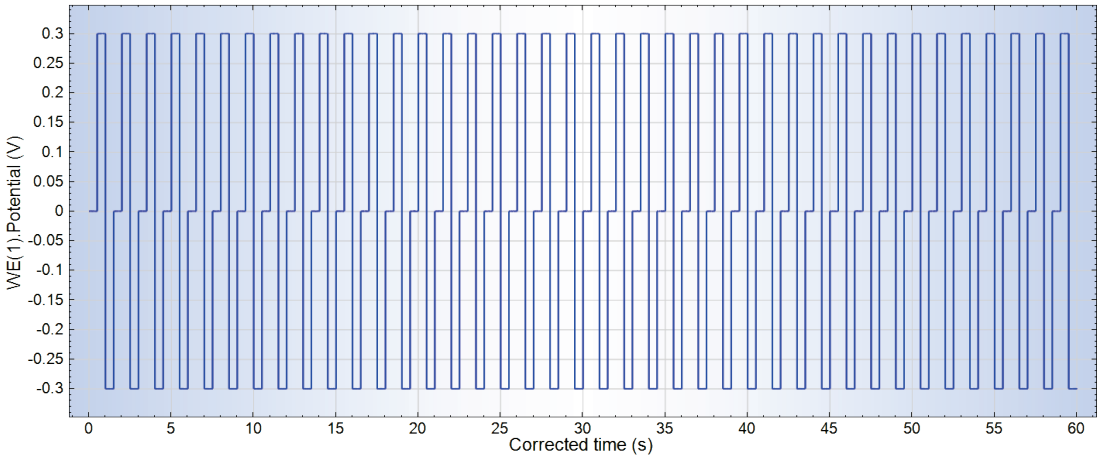


Figure 200 – The potential profile obtained with a 60 s chrono methods command

Note: to ensure that the timing of all the events during the chrono methods command is as accurate as possible, the Autolab cannot display the measured data points in real time. While the chrono methods command is running, the Autolab display will indicate a busy timer in the lower left angle (see Figure 201). When the chrono methods measurement finishes, the rest of the procedure will be executed.

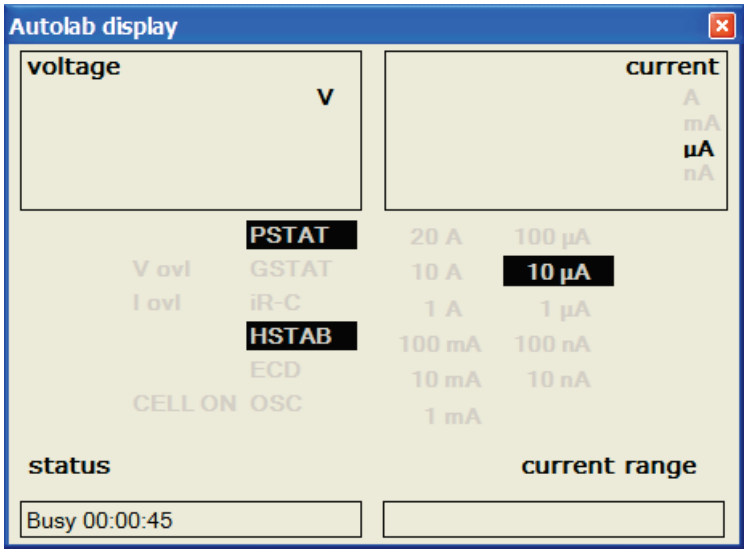


Figure 201 – The Autolab display window with the Busy timer in the lower left corner

SCAN250 & SCANGEN in combination with the ADC164

NOVA 1.3 now supports the combination of the SCAN250/SCANGEN with the ADC164. The SCAN250 was previously only available in combination with the ADC750 or the ADC10M.

A dedicated command, *CV linear scan,* is available from the measurement group. This command performs a linear scan cyclic voltammogram with the SCAN250 or the SCANGEN module while the electrochemical signals are sampled using the ADC164.

The *CV linear scan high speed* command can be used to perform a cyclic voltammogram with the SCAN250 or the SCANGEN module while the current and the potential are sampled using a high speed ADC, either the ADC750 or the ADC10M.

New linking behavior

Links are an important component of the procedure building process. Links are used in Nova to establish a dynamic relationship between two or more parameters or signals.

To provide a clear overview of the linked parameters or signals, Nova 1.3 now highlights a link whenever one of the linked items is selected (see Figure 202). Unselected links are displayed in light grey color.

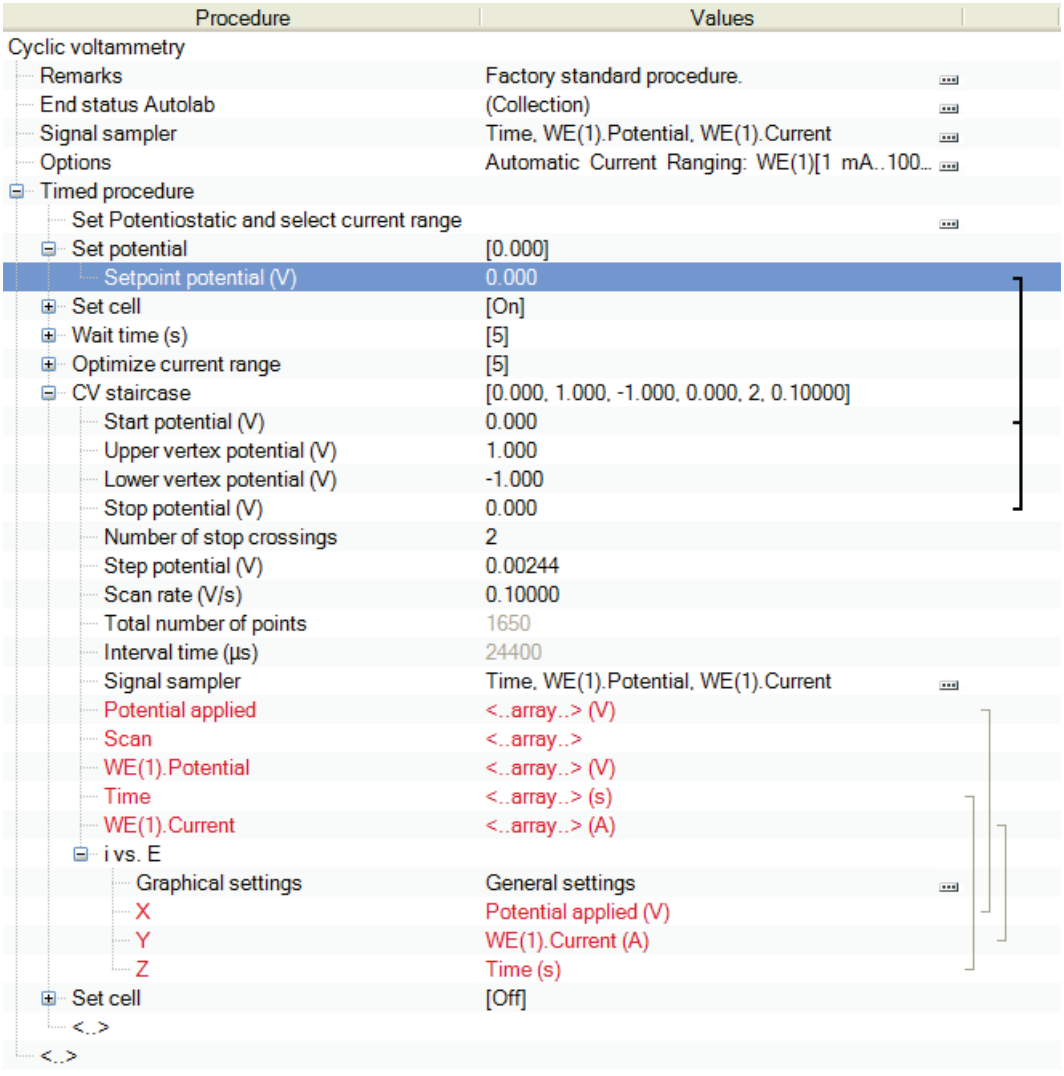


Figure 202 – Links are highlighted whenever a linked parameter or signal is selected

Note: linking and unlinking is now available through the right mouse button.

Printable links

The print procedure option, available from the File menu can now be used to print the visible links along with the rest of the procedure (see Figure 203). All the links will be printed on the right hand side. A print preview is available from the File menu.

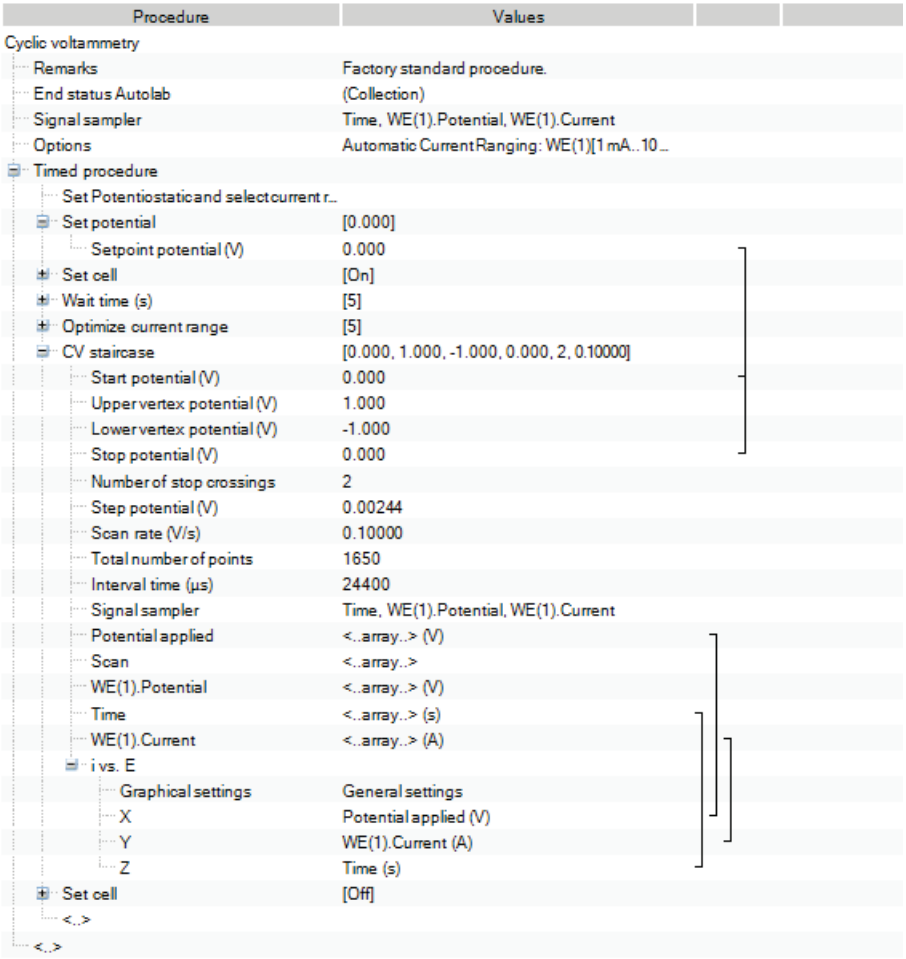


Figure 203 – Print preview of the cyclic voltammetry procedure with the links on the right hand side

Note: only the visible links will be printed.

Maintaining reverse compatibility

This version of NOVA introduces a large number of changes that affect the way the software reads and writes data files. In order to ensure backwards compatibility with the previous release version, conversion tools are provided.

Previously recorded data sets, obtained with NOVA 1.2, need to be converted using these tools before the data and the procedures can be used by NOVA 1.3. This section describes how to use the conversion tools.

The main difference between version 1.2 and 1.3 is that the former uses a single file database storage system whereas the latter uses a multiple file database storage. This means that data sets obtained with NOVA 1.2 have first to be extracted from the database as individual NOVA 1.2 *.nox* files (export phase). The Nova 1.2 *.nox* files can then be converted into *.nox* files which can be used by NOVA 1.3 (conversion phase). The two steps are schematically summarized in Figure 173.

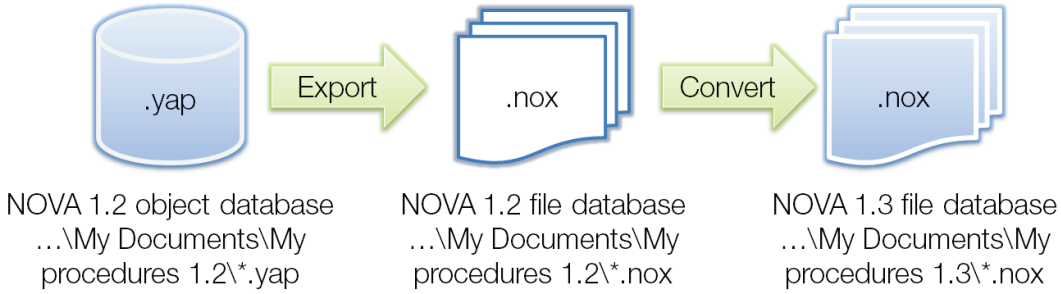


Figure 204 – Schematic view of the NOVA 1.2 to NOVA 1.3 conversion process

After installing NOVA 1.3, start the *Export databases 1.2 to files* application (Start menu – Programs – Autolab – Tools). This will start the export application, which will display the contents of the default folder containing the NOVA 1.2 databases (My Documents – My Procedures 1.2). All the NOVA 1.2 databases in this folder will be displayed (see Figure 174).

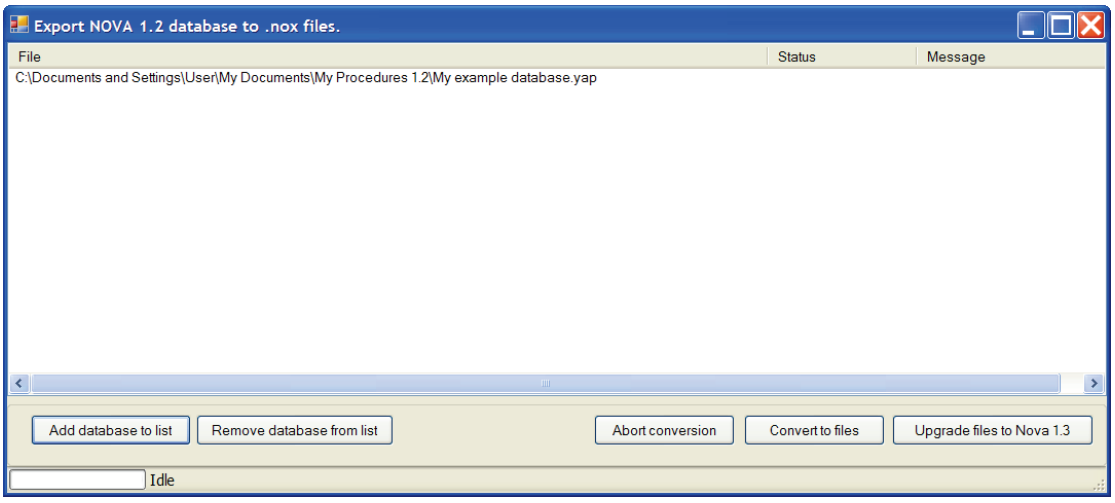


Figure 205 – The contents of the My Procedures 1.2 folder are displayed in the Export application

Using the *Add database to list* and the *Remove database from the list* buttons, databases can be added or removed from the list.

The conversion involves two steps. The first conversion step converts the selected database(s) to individual *.nox* files and the second conversion step converts the NOVA 1.2 files to NOVA 1.3 files.

Having selected the databases that have to be converted from the 1.2 format to the 1.3 format, click the *Convert to files* button to start the first conversion step (see Figure 206). Depending on the number of databases and the size of the selected databases, this step could take several minutes.

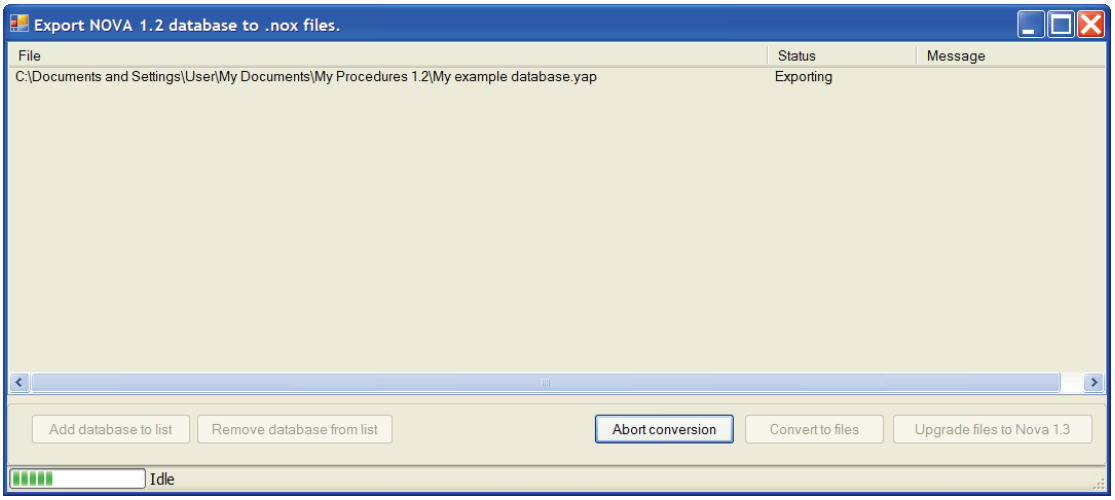


Figure 206 – During the first conversion step, the contents of the selected database(s) are exported to individual .nox files

During the conversion step, the progress is displayed in real time. When the first step is finished, the extracted files can be upgraded to the NOVA 1.3 file format (see Figure 207).

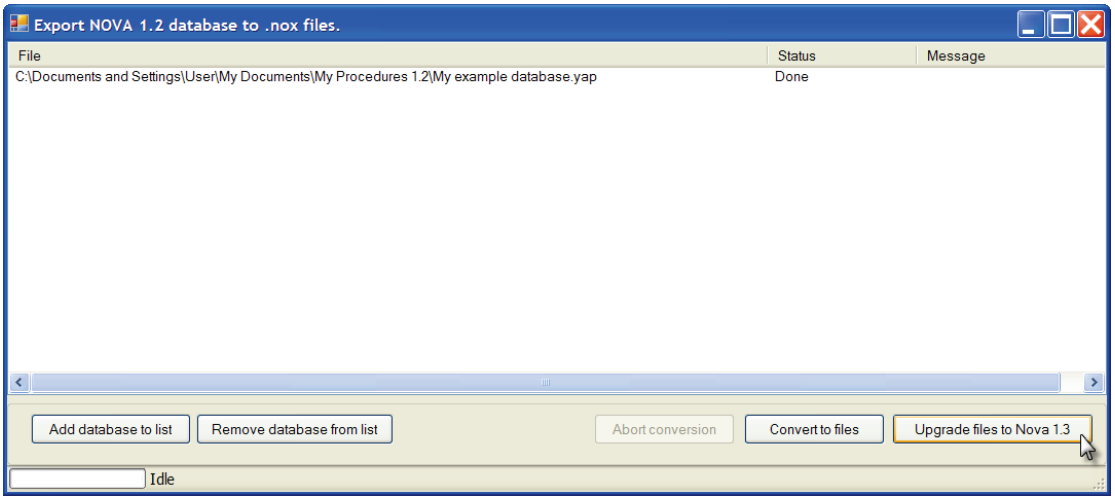


Figure 207 – When the extraction process is finished, the files can be upgraded to the NOVA 1.3 file format

Note: the original databases will not be destroyed, which means that you can still access the data from NOVA 1.2.

Click the Upgrade files to NOVA 1.3 button to continue. The Export application will close and the Upgrade application will be loaded. The exported *.nox* files will be displayed in the list (see Figure 208).

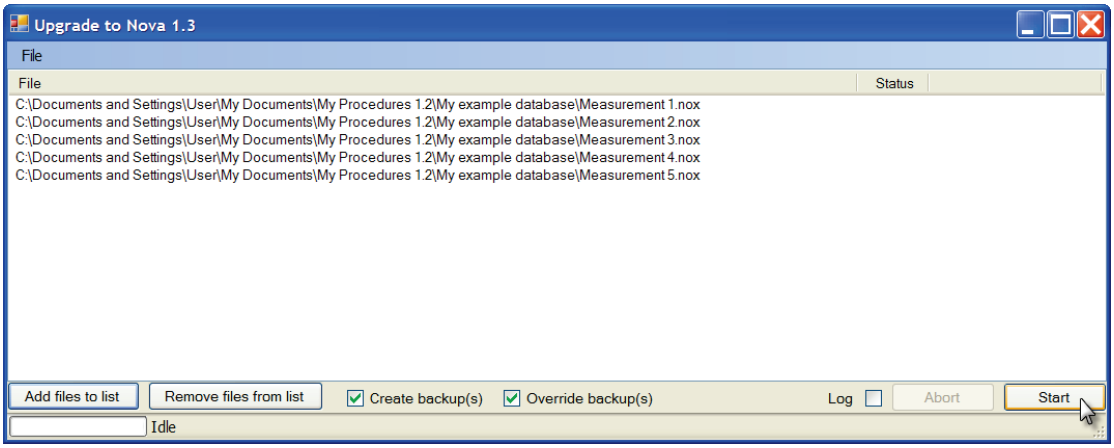

Upgrade to Nova 1.3
File
File
Status
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 1.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 2.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 3.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 4.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 5.nox
Add files to list
Remove files from list
Create backup(s)
Override backup(s)
Log
Abort
Start
Idle

Figure 208 – The upgrade application displays the available *.nox* files in NOVA 1.2 format

Using the *Add files to list* and the *Remove files from the list* buttons, individual *.nox* files can be added or removed from the list.

Click the Start button to initiate the conversion to the NOVA 1.3 file format. It is possible to create a backup of the source files and to overwrite the backup files if they are already found in the source folder. It is also possible to create a log file, which can be useful if the conversion fails.

During the upgrade step, the progress is displayed in real time (see Figure 176).

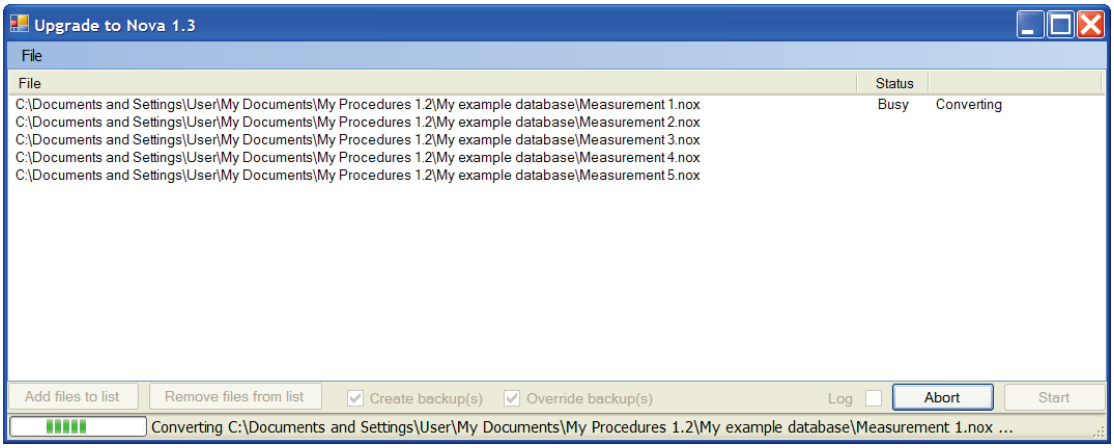

Upgrade to Nova 1.3
File
File
Status
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 1.nox
Busy
Converting
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 2.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 3.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 4.nox
C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 5.nox
Add files to list
Remove files from list
Create backup(s)
Override backup(s)
Log
Abort
Start
Converting C:\Documents and Settings\User\My Documents\My Procedures 1.2\My example database\Measurement 1.nox ...

Figure 209 – The upgrade application converts every .nox file in the list from the NOVA 1.2 format to the NOVA 1.3 format

When all the .nox files have been processed, they will be compatible with the NOVA 1.3 format (see Figure 177).

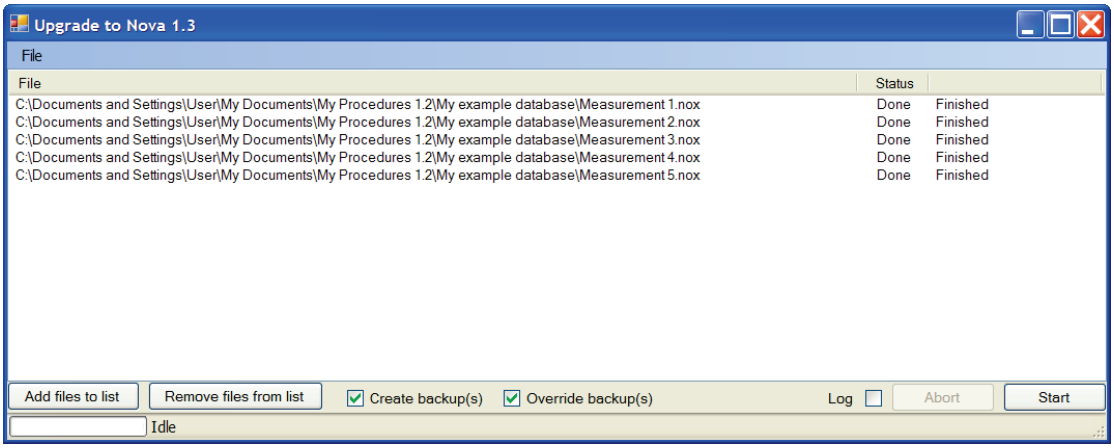


Figure 210 – When the upgrade application has finished, the converted .nox files will be ready for NOVA 1.3

Note: if the location of the NOVA 1.2 source database is the My Documents\My Procedures 1.2, the converted files will be automatically copied to the My Documents\My Procedures 1.3 folder. If the source database is located in another folder, the same folder will be used as location for the NOVA 1.3 .nox files.

Diagnostics

NOVA 1.3 introduces a new version of the diagnostics tool. This tool is provided as a stand alone application and can be accessed from the start menu, in the Autolab group (Start menu – All programs – Autolab – Tools).

The diagnostics tool can be used to troubleshoot an instrument or perform individual tests to verify the correct operation of the instrument. It requires the standard dummy cell, with the WE lead (and the S lead, if present) connected to the (a) circuit of the cell. It also requires a BNC cable connected between the ADC164 channel 2 to the DAC164 channel 2 on the front panel of the instrument.

In order to perform the tests, the diagnostics tool must be configured according to the instrument type. The configuration of the diagnostics tool is done using the select menu (see Figure 211).

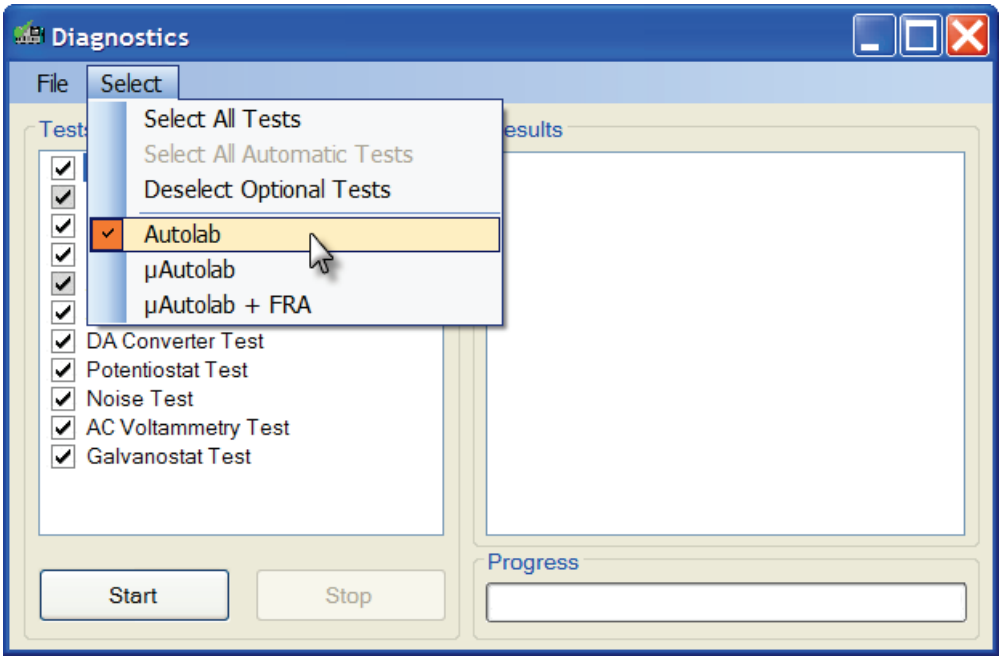


Figure 211 – Setting the hardware selection in the diagnostics tool from the Select menu

For all the PGSTATs, the Autolab setting should be selected. For the µAutolab and the µAutolab with FRA module, a specific setting should be used instead.

Pressing the start button will initiate all the selected tests. The connection with the instrument will be established by the diagnostics tool during the Embedded Processor Test.

During the test, the progress will be displayed and a successful test will be indicated by a green symbol (see Figure 212).

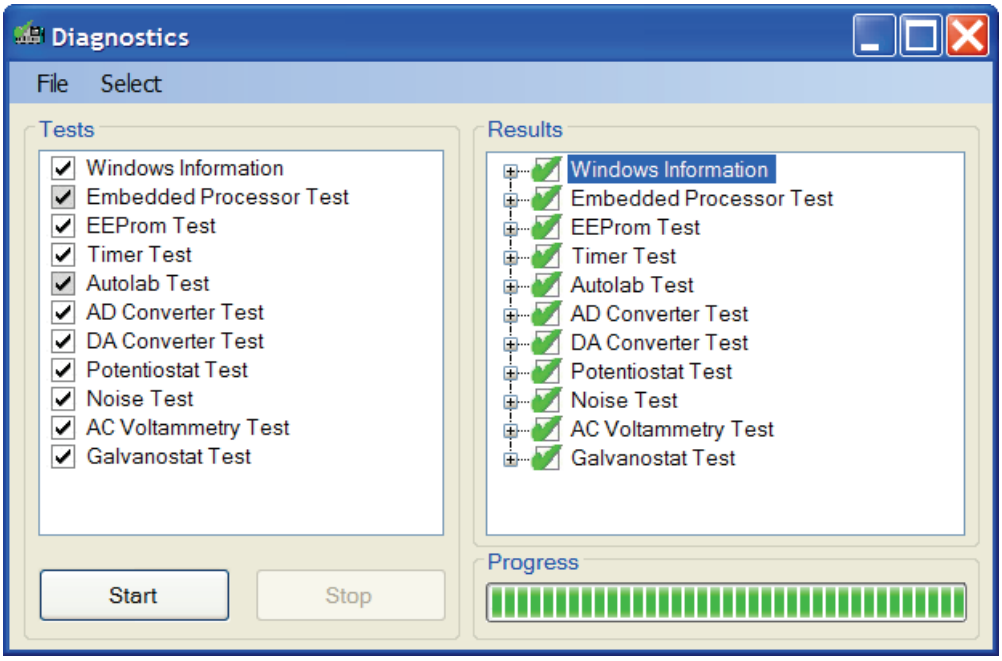


Figure 212 – The diagnostics report after all the tests have been performed successfully

If all the tests succeed, the instrument is working correctly. It is possible to verify the results of a specific test by clicking open the details in the diagnostics tool (see Figure 213).

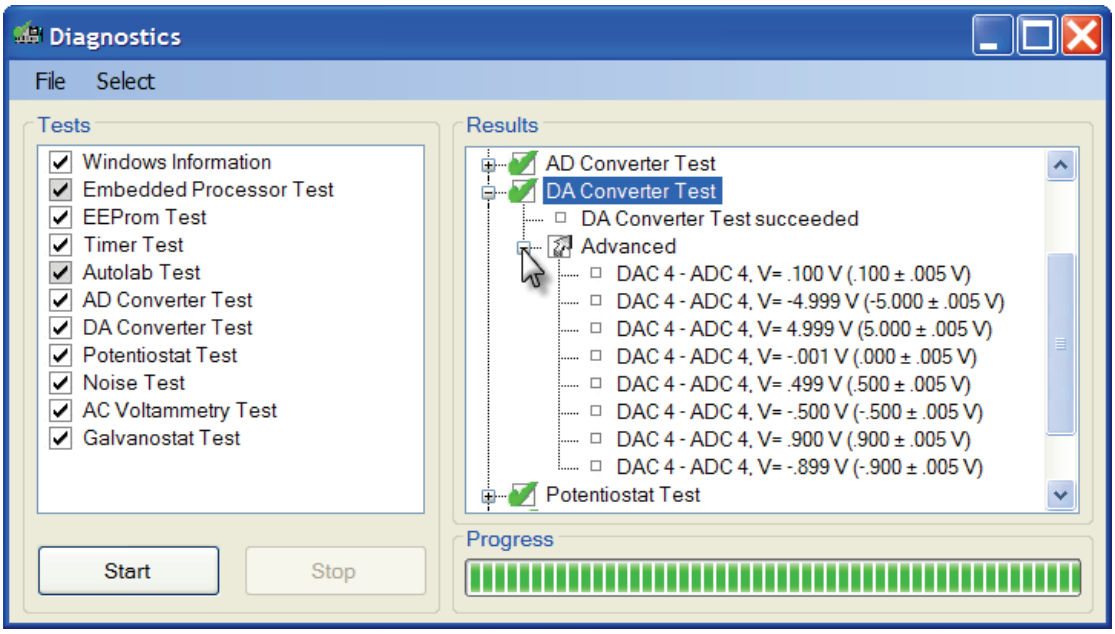

Diagnostics
File
Select
Tests
Windows Information
Embedded Processor Test
EEProm Test
Timer Test
Autolab Test
AD Converter Test
DA Converter Test
Potentiostat Test
Noise Test
AC Voltammetry Test
Galvanostat Test
Results
AD Converter Test
DA Converter Test
DA Converter Test succeeded
Advanced
DAC 4 - ADC 4, V= .100 V (.100 ± .005 V)
DAC 4 - ADC 4, V= -4.999 V (-5.000 ± .005 V)
DAC 4 - ADC 4, V= 4.999 V (5.000 ± .005 V)
DAC 4 - ADC 4, V= -.001 V (.000 ± .005 V)
DAC 4 - ADC 4, V= .499 V (.500 ± .005 V)
DAC 4 - ADC 4, V= -.500 V (-.500 ± .005 V)
DAC 4 - ADC 4, V= .900 V (.900 ± .005 V)
DAC 4 - ADC 4, V= -.899 V (-.900 ± .005 V)
Potentiostat Test
Progress
Start
Stop

Figure 213 – The diagnostics tool displays the details of all the tests

If one or more of the tests fails, a red symbol will be used to indicate which test failed and what the problem is. Figure 214 shows the output of the diagnostics tool when the test is performed with a faulty USB connection.

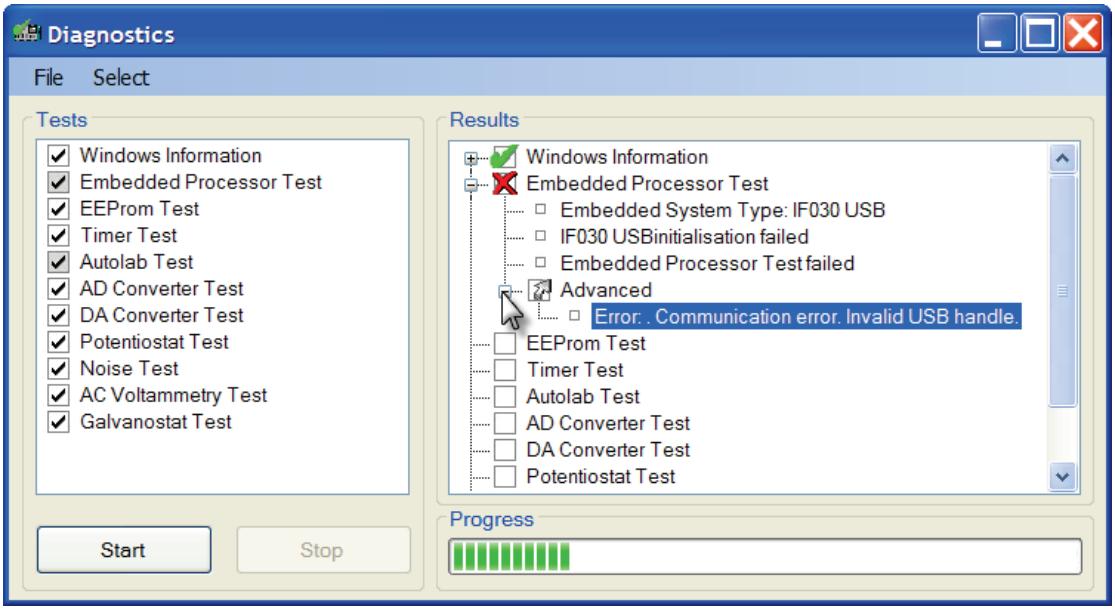


Figure 214 – A failed test will be indicated in the diagnostics tool

It is possible to print the test report or to save it as a text file by using the File menu and selecting the appropriate action (see Figure 215).

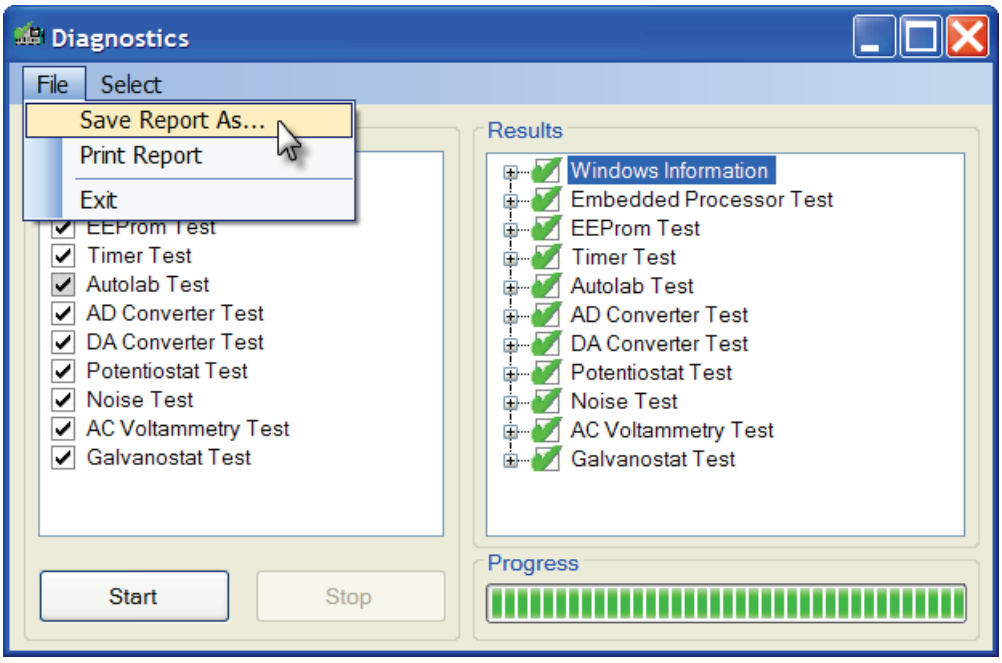


Figure 215 – It is possible to save or print the diagnostics report

Signal set(s) for each measurement command

It is now possible to define one or more signal set for each measurement command which will be created during the measurement. Each measurement command has a *default* signal set, which can be edited.

The signal set(s) added to a measurement command can use any electrochemical signal defined in the sampler of the command. Figure 216 shows the default

signal set used for the CV Staircase command. The signal set, *i vs. E*, uses the following electrochemical signals:

- X – Potential applied (V)
- Y – WE(1).Current (A)
- Z – Time (s)

The definition of the electrochemical signals used in the signal set is achieved using links.

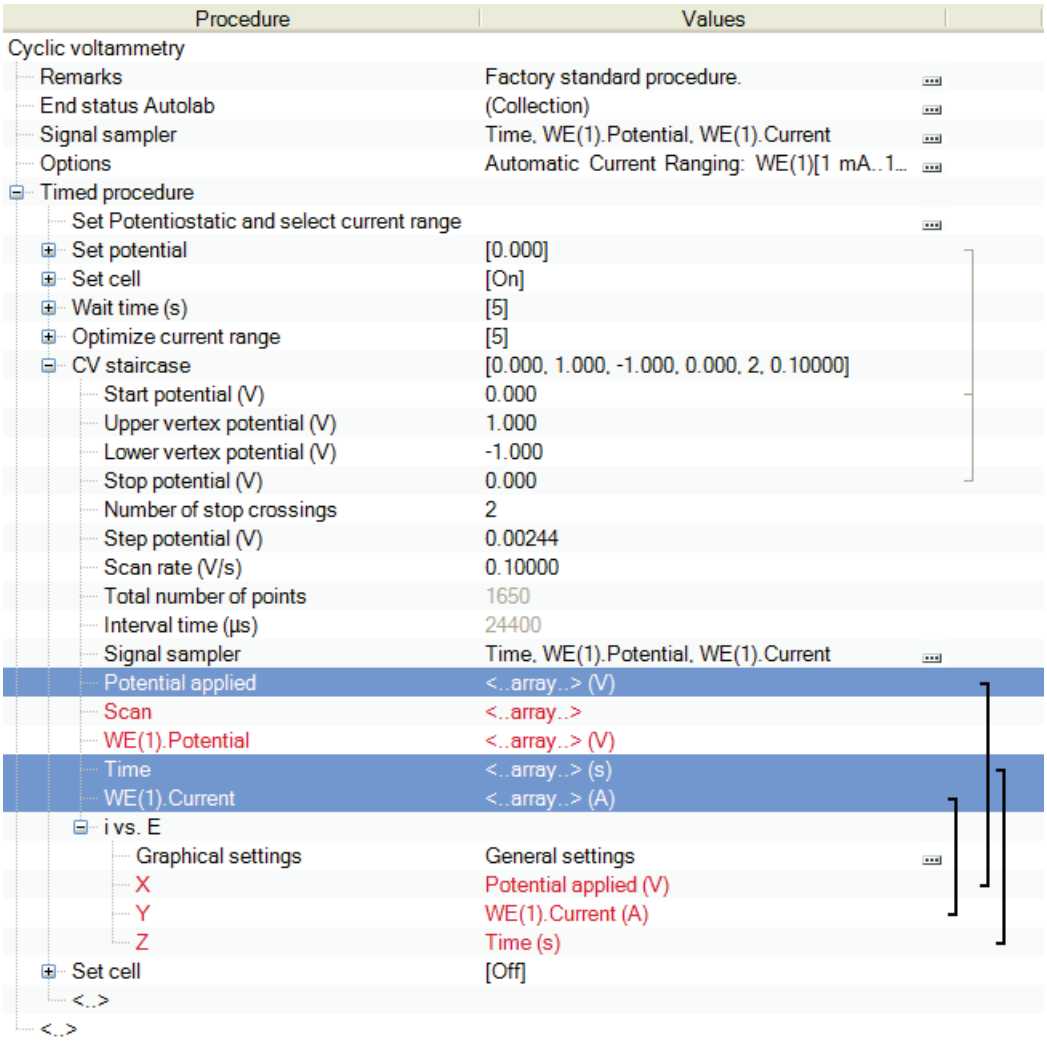


Figure 216 – The Cyclic voltammetry procedure with the default Signal set of the CV Staircase command

The signal set(s) added to a measurement command of a procedure define how the measured data is displayed in real time, during the measurement. For the CV Staircase command, the WE(1).Current signal will be plotted against the Potential applied in real time.

If the links are changed, for example by replacing the Potential applied by the Time, the data will be plotted differently during the measurement (see Figure 217).

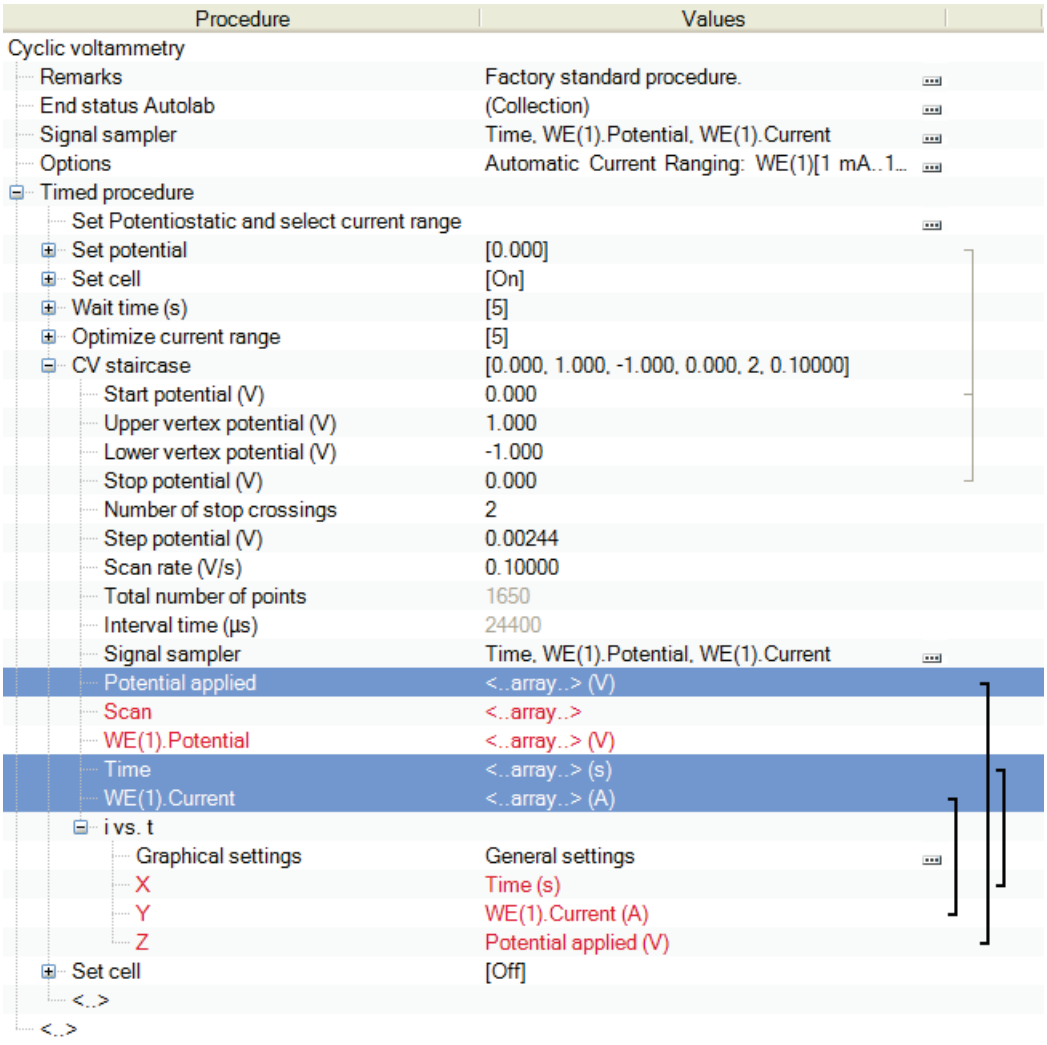


Figure 217 – Modifying the links used for the Signal set will change the way the data is displayed during the measurement

More than one signal set in the measurement view

It is possible to add more than one signal set to a measurement command. Each signal set will be displayed in the measurement view, which means that it is now possible to plot more than one signal in real time.

For the Cyclic voltammetry procedure, this can be achieved by dragging a Signal set command from the command browser and drop on the CV Staircase command (see Figure 218).

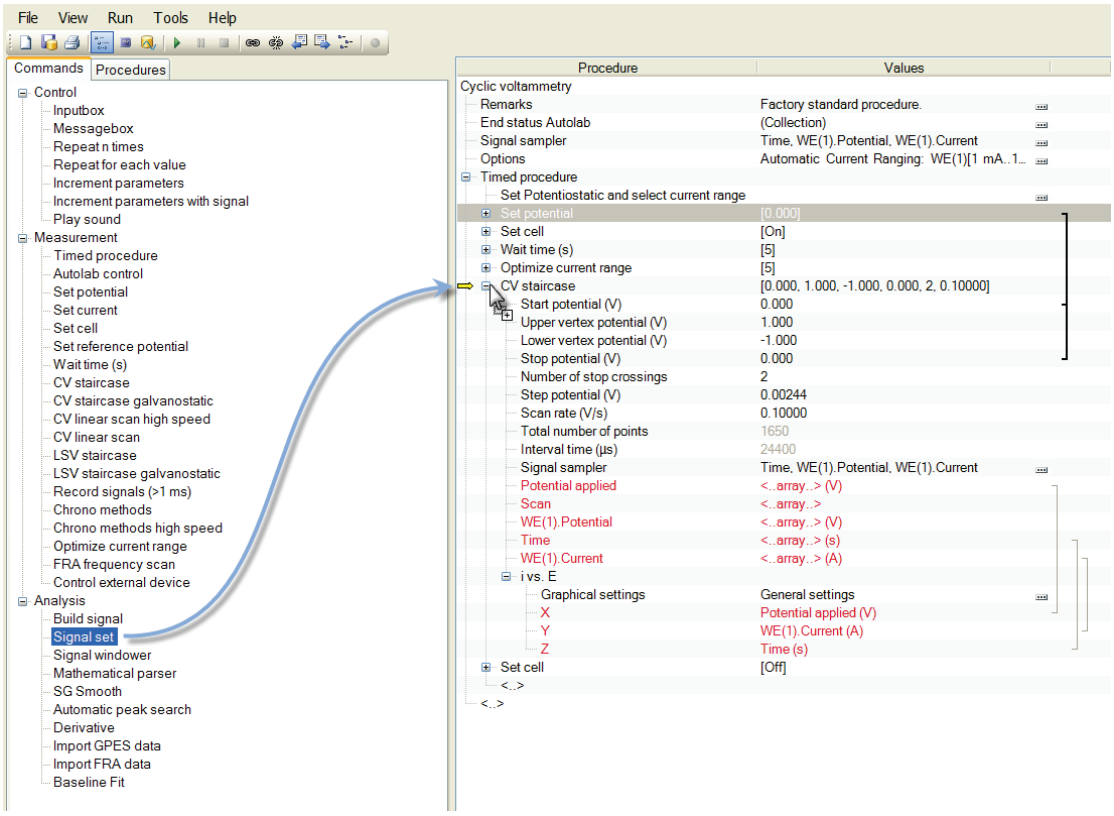


Figure 218 – Adding a Signal set command to a measurement command can be done by dragging

A new signal set command will be available for the CV Staircase command (see Figure 219). It is possible to select which electrochemical signals to use for this new signal set, by linking the available signals of the CV Staircase to the X, Y and Z inputs of the signal set command.

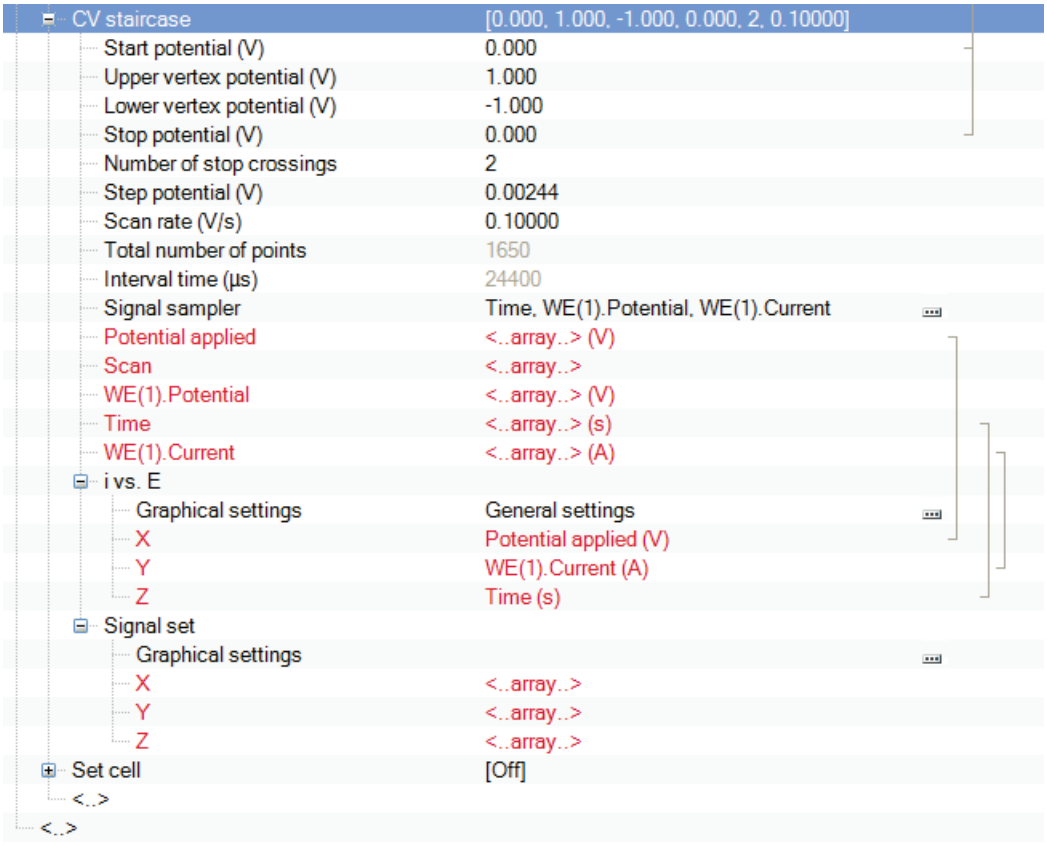


Figure 219 – The new signal set is added to the CV Staircase command

Setting up the signal set(s), more than one plot can be displayed in real time. Figure 220 shows an example in which two signals are plotted in the measurement view during the measurement.

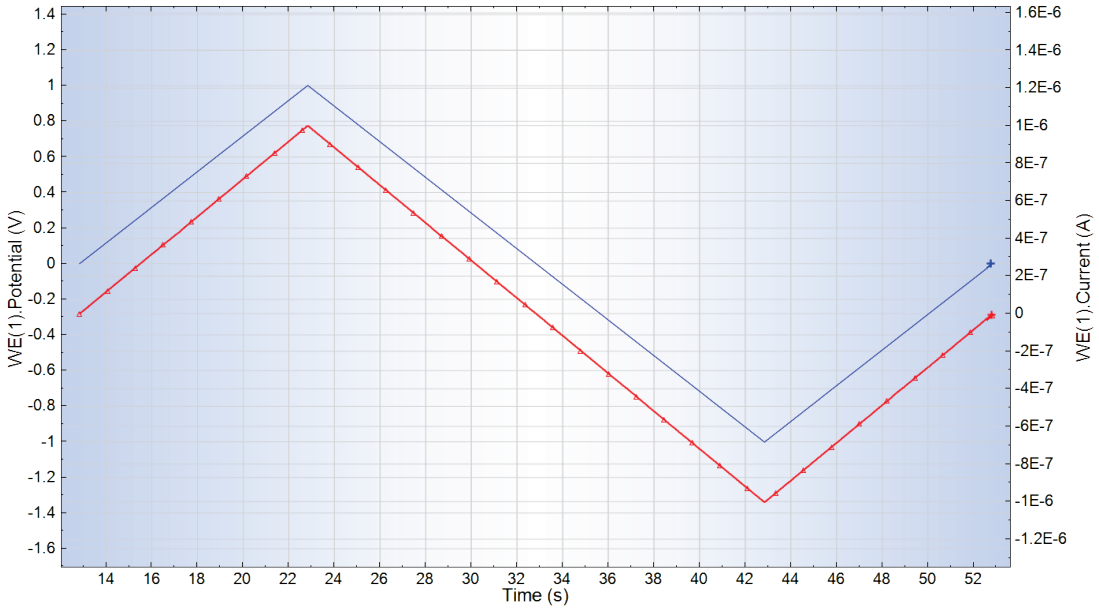


Figure 220 – Real time plot for the Cyclic voltammetry procedure showing two signals plotted at the same time. The blue curve corresponds to the WE(1).Potential (left axis) and the red curve corresponds to the WE(1).Current (right axis)

Clear plot during measurement

The clear measurement plot button in the toolbar is now available during the measurement. If this button is pressed during a measurement, the plot will be cleared, even if a measurement is ongoing. The plotting of the data will resume after the plot is cleared.

Manual rescale during measurement

In NOVA 1.3, it is possible to disable the automatic rescaling during a measurement. Any action changing the scaling of the plot during a measurement (for example, zooming in or out or changing the scaling of one of the axes), will interrupt the automatic rescaling feature of NOVA. Pressing the F4 key will resume automatic rescaling.

Mathematical parser as a command

The *Mathematical parser* command is available from the Analysis group in the command browser. This command can be used to perform a calculation, during the measurement or at the end of it.

The mathematical parser command requires a user defined mathematical formula and a source electrochemical signal for each variable in the mathematical expression.

Figure 221 shows a typical example of the Mathematical parser command. In this case, the Mathematical parser command has been added at the end of the procedure.

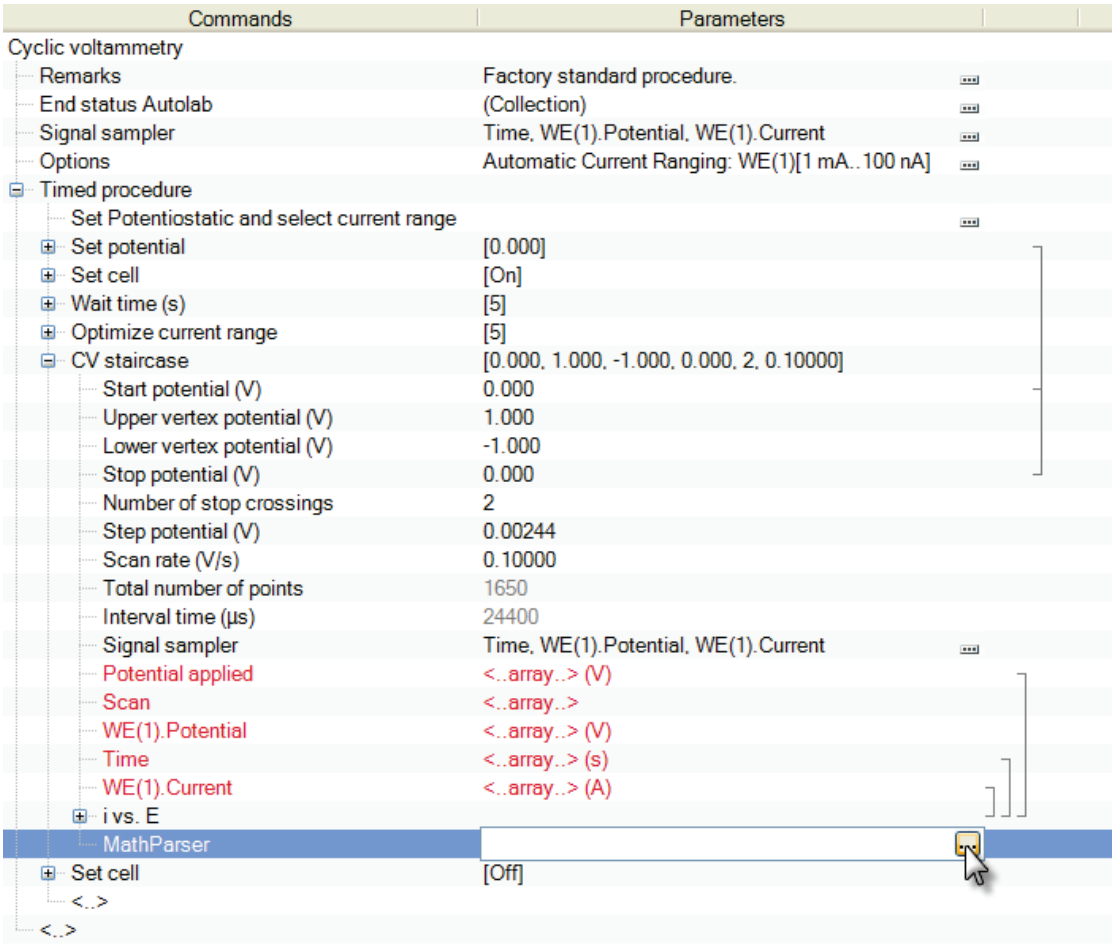


Figure 221 – The mathematical parser command added to the Cyclic voltammetry procedure

To use this command, click the ... button located on the right-hand side. This will open the Expression builder window, in which the mathematical function can be created (see Figure 222).

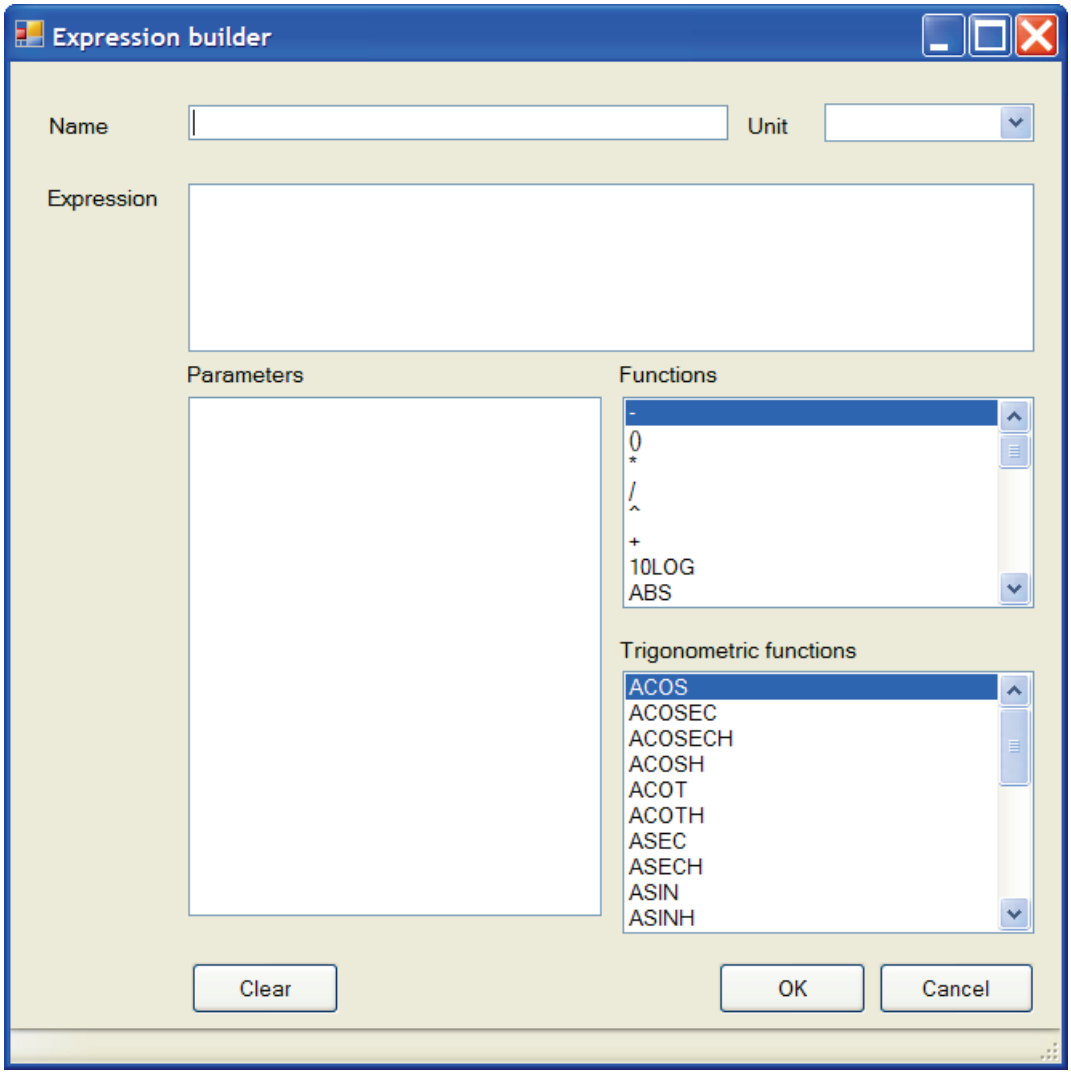


Figure 222 – The expression builder window

The following items are required:

- **Name** – this is the name of the electrochemical signal generated by the calculation.
- **Unit** – this is the unit of the calculated signal.
- **Expression** – this is the mathematical expression used for the calculation. The functions provided in the two lists on the right hand side of the expression builder window can be used to build the expression.

The unit group can be used to assign a unit to the calculated electrochemical signal. The unit can be selected from the drop-down list or it can be entered manually.

The parameters field, which is updated once a formula has been entered, provides a list of all the variables that are used in the calculation. In Figure 223, the expression builder is used to calculate the logarithmic value of the absolute value of the current. The formula has only one parameter, the *Current* (see Figure 223).

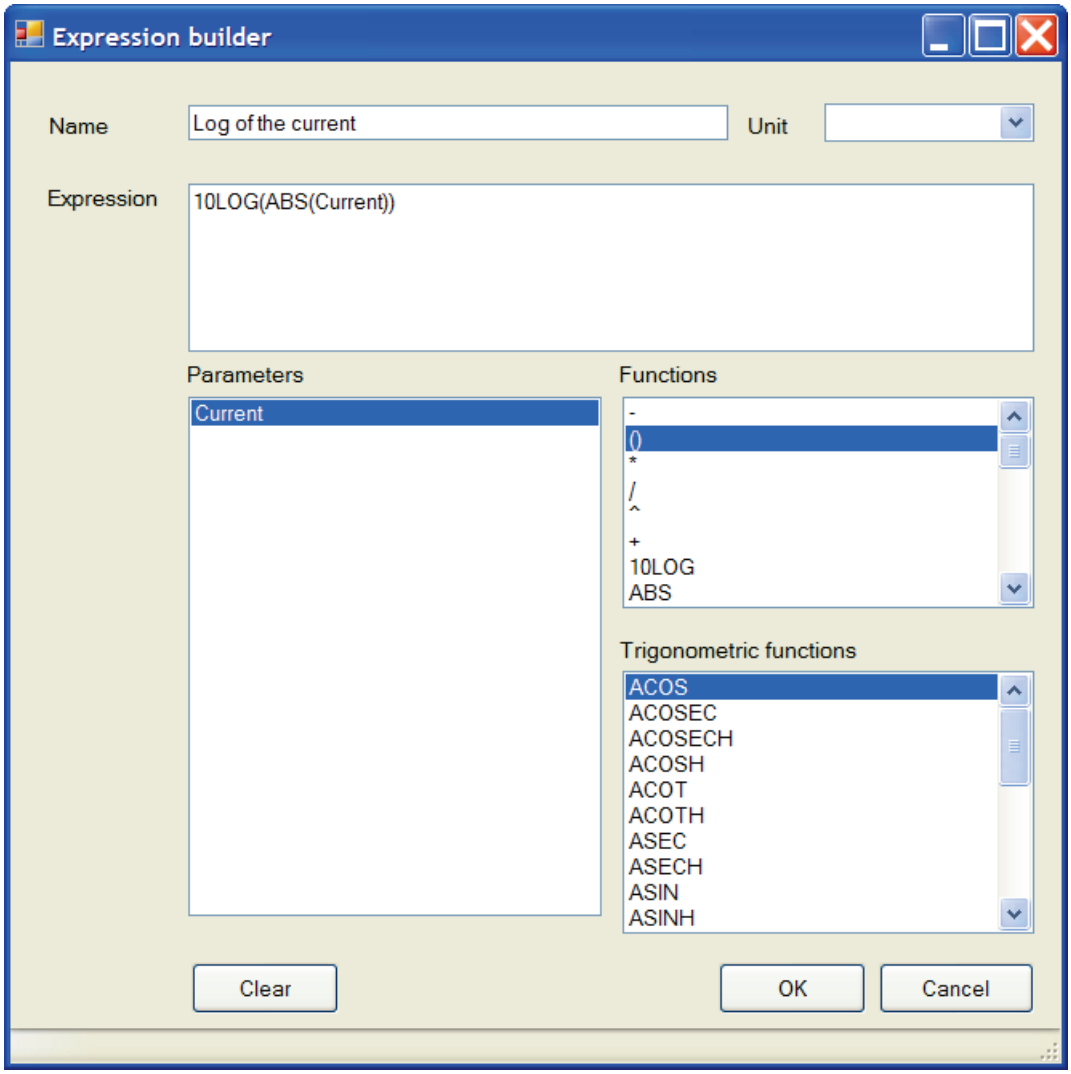


Figure 223 – The expression builder and the formula used in the Mathematical parser

When the mathematical expression has been entered, the expression builder can be closed by clicking the OK button.

The Mathematical parser command will be updated (see Figure 224). A list of parameters will be displayed under the Mathematical parser command. Each of these parameters has to be linked to the source electrochemical signal that has to be used in the calculation.

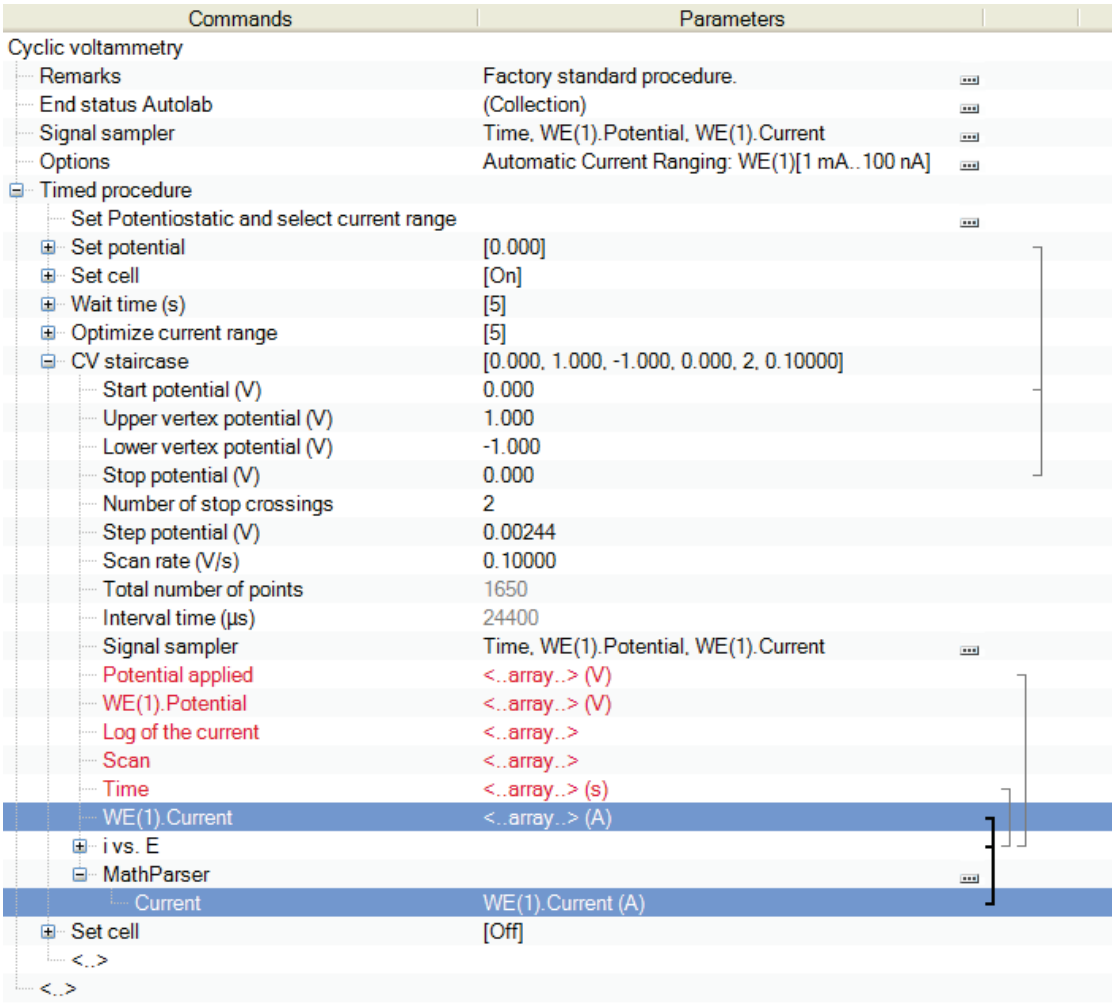


Figure 224 – The parameters of the mathematical parser command have to be linked to the source electrochemical signals

In the example shown in Figure 224, the *Current* parameter has been linked with the WE(1).Current electrochemical signal. At the end of the measurement, the values of the WE(1).Current will be used in the predefined calculation and a new electrochemical signal, *Log of the current*, will be added to the data set. This calculated signal will then be available for data analysis.

Improved Autolab control interface

The *Autolab control* command is available from the measurement group in the commands browser. This command defines hardware settings of the instrument, like the selected current range, the cell status, the bandwidth of the potentiostat/galvanostat, etc…

The Autolab control command is already available in NOVA 1.2. This version of NOVA introduces some user interface changes. To use this command, click on the … button located on the right hand side (see Figure 225).

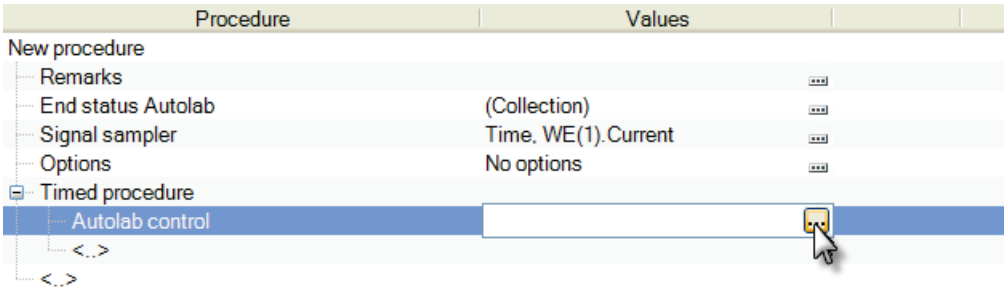


Figure 225 – Opening the Autolab control user interface

Figure 226 shows a typical view of the Autolab control interface. For each hardware module with manual settings, a list of items are available (in Figure 226, the settings for WE(1), WE(2) and DIO are available).

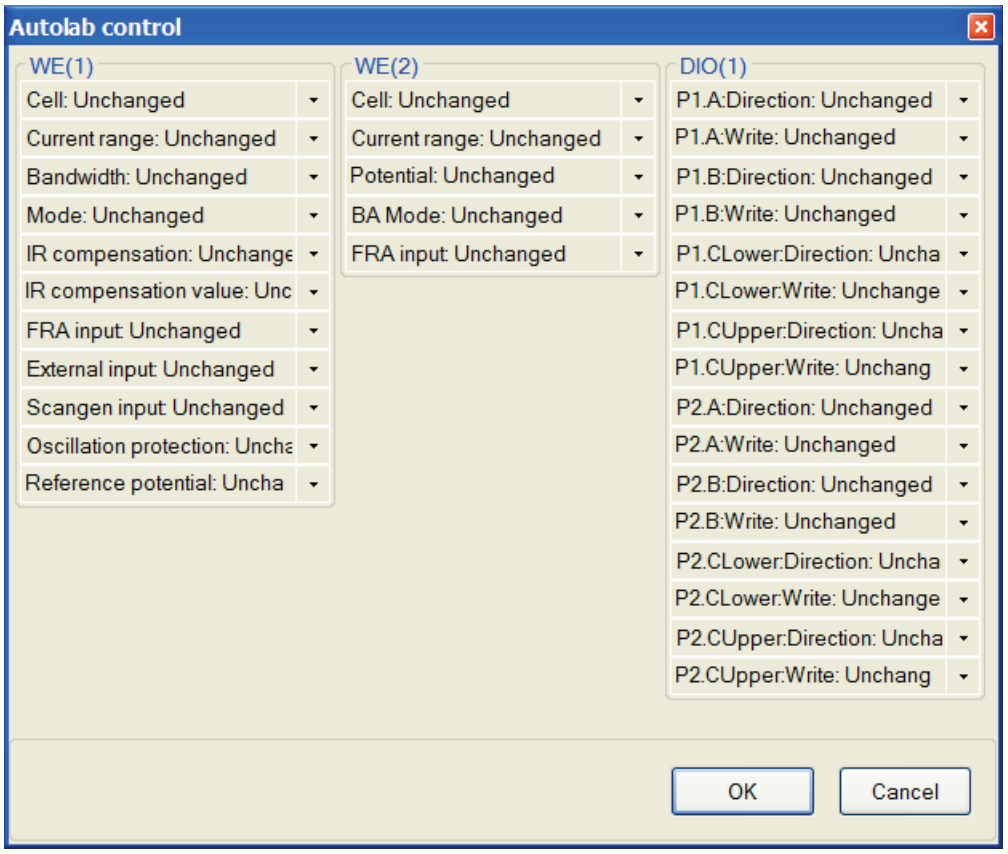


Figure 226 – A typical Autolab control interface window

The available settings for each item can be selected from a drop-down list (see Figure 227). The default status of each item is **Unchanged**, which means that the settings of the instrument will not be changed, unless it is required by the user.

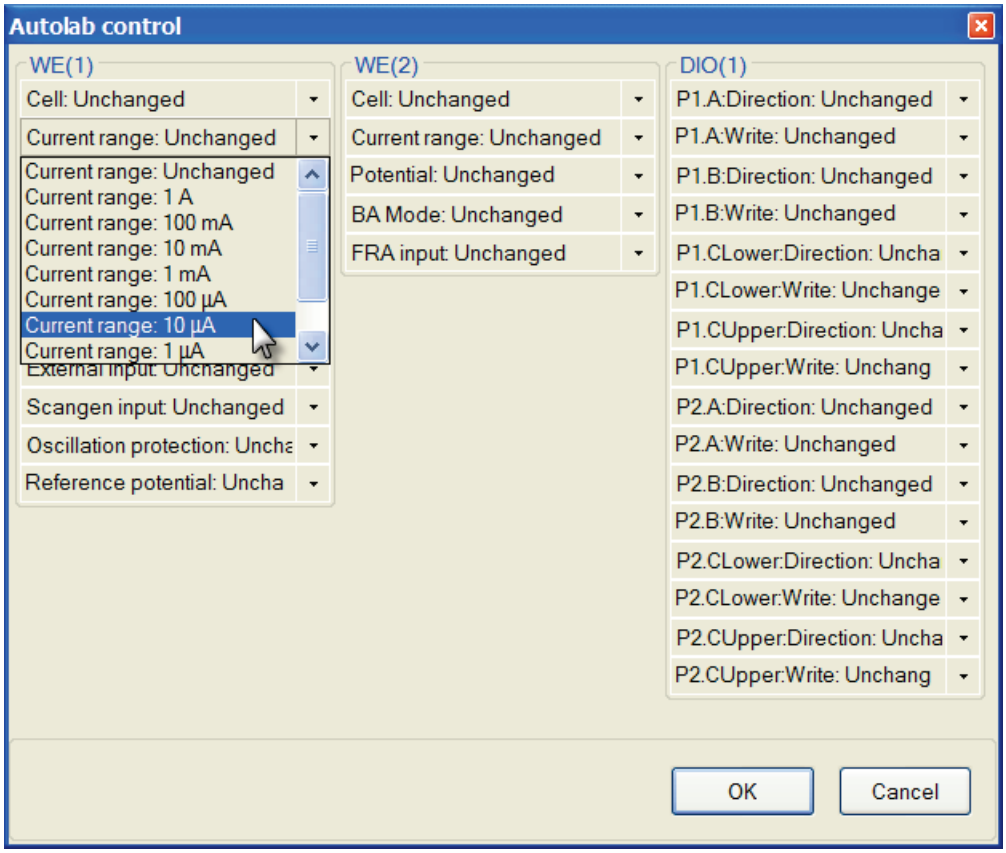


Figure 227 – Changing the settings can be done using the drop-down lists

To change a setting, select the new value from a drop-down list. Figure 228 illustrates the change of one of the hardware settings. Using the drop-down lists, the active current range for the WE(1) can be set to 10 µA.

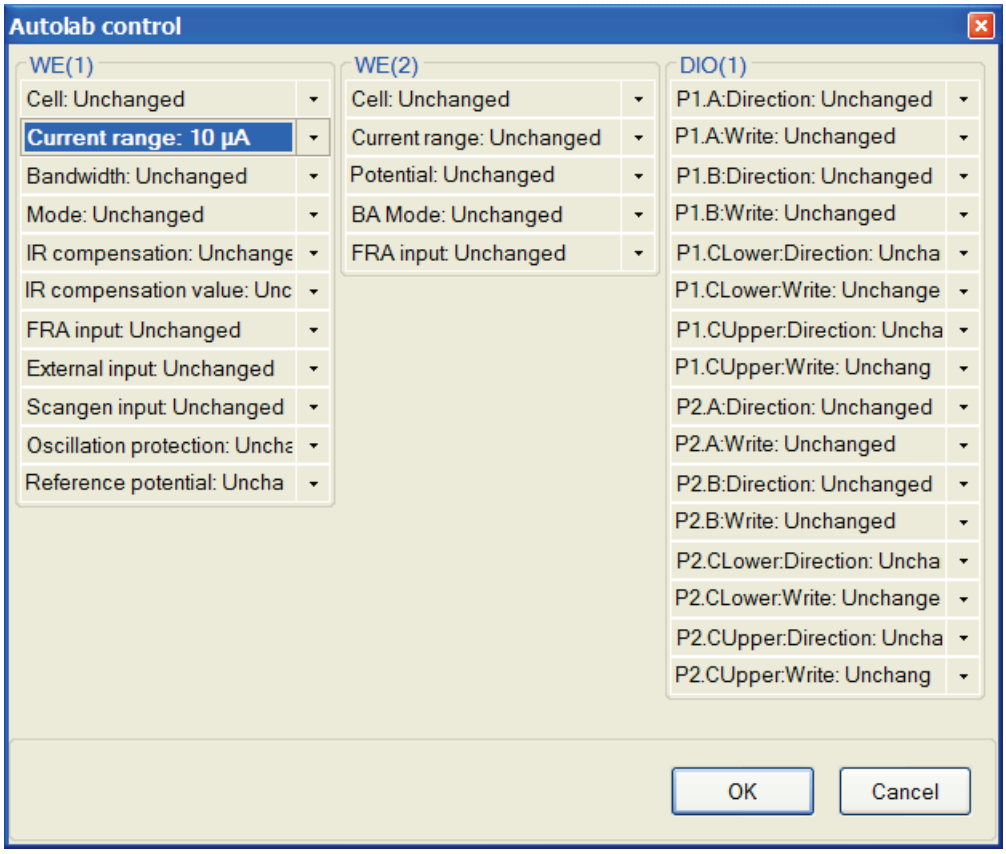


Figure 228 – The changes in the Autolab control command are highlighted

Note: the Autolab control command only displays the settings of the hardware modules defined in the hardware setup.

OCP integration

Open circuit potential measurements are now easier compared to the previous versions of NOVA. A new command, *OCP determination*, is now available from the measurement group in the commands browser. This command samples the WE(1).Potential during a pre-defined time (see Figure 229).

Figure 229 – The OCP determination command

The OCP determination command has the following parameters:

- Signal sampler: defines the signals that are sampled during the OCP determination (WE(1).Potential and Time are the default settings)
- Maximum time (s): defines the maximum duration of the OCP determination
- dE/dt limit: defines an optional cutoff value for the derivative of the OCP (if this value is set to 0, the dE/dt limit is not used)
- Use average OCP: yes/no – this settings defines whether the moving average the OCP values, measured during 5 seconds, should be used in the determination of the OCP or if the last measured OCP value should be used instead

The *OCP determination* command comes with a signal set, which displays the WE(1).Potential versus time during the measurement. A second window is also displayed during the measurement, displaying real time information about WE(1).Potential and dE/dt (see Figure 230).

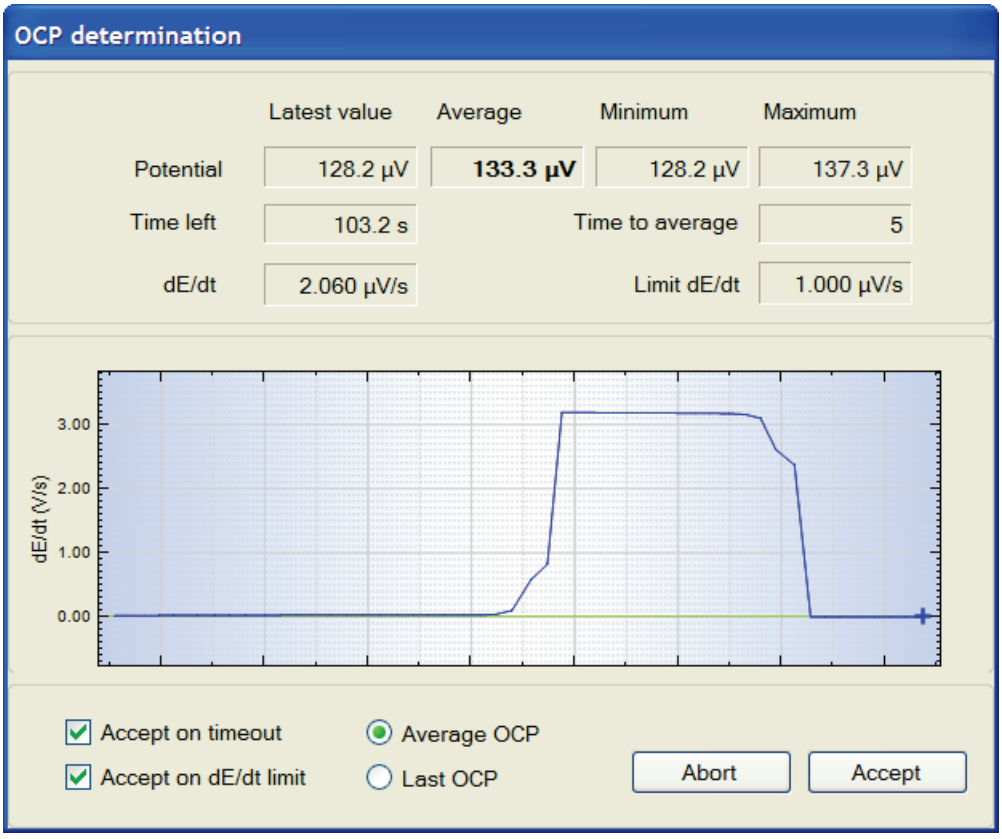


Figure 230 – The OCP determination window displayed during the measurement

During the OCP determination, it is possible to check or uncheck the 'Accept on timeout' and 'Accept on dE/dt limit' options. It is also possible to switch from the average OCP to the last measured OCP.

The minimum and maximum values represent the lowest and highest value of the WE(1).Potential measured during the OCP determination. The green line plotted in the OCP determination window represents the dE/dt limit.

Note: it is possible to press the Accept button to stop the OCP determination and use the last value of the WE(1).Potential as the OCP.

Set reference potential command

A new *Set reference potential* command is available from the measurement group in the command browser. This command can be used to apply any offset to the potential applied on the working electrode (WE(1)), in potentiostatic mode. This command can be used in combination with the OCP determination command, to apply all the potentials with respect to the OCP (see Figure 231).

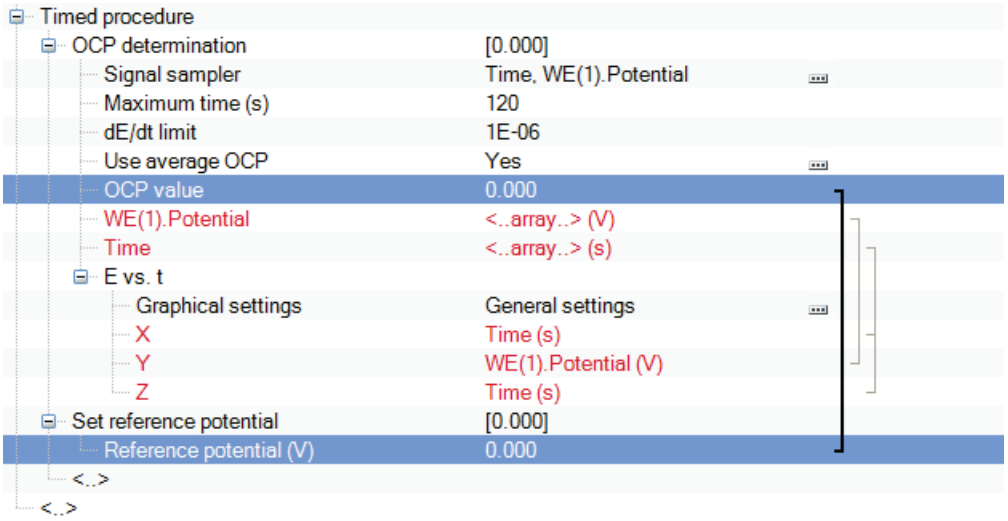


Figure 231 – Linking the OCP value with the Set reference potential will force NOVA to apply all the potential values with respect to OCP

The same command can be used to correct the potential of the working electrode with a user-defined offset. This offset will be added to all the potential values in the procedure. This can be useful if the experimental settings are defined relative to a different reference electrode than the one in use.

Note: in this case, it is not required to link the Reference potential parameter.

Import FRA data command

An *Import FRA data* command has been added to the analysis group of the command browser. This command is similar to the *Import GPES* data. It allows importing data files obtained with the FRA software into the NOVA 1.3 database.

Figure 232 illustrates the use of the Import FRA data command. The parameter of the command is the location of the .dfr file. The command generates a Nyquist plot and a Bode plot automatically.

Note: the Import FRA data command can be used even if there is no instrument connected to the computer.

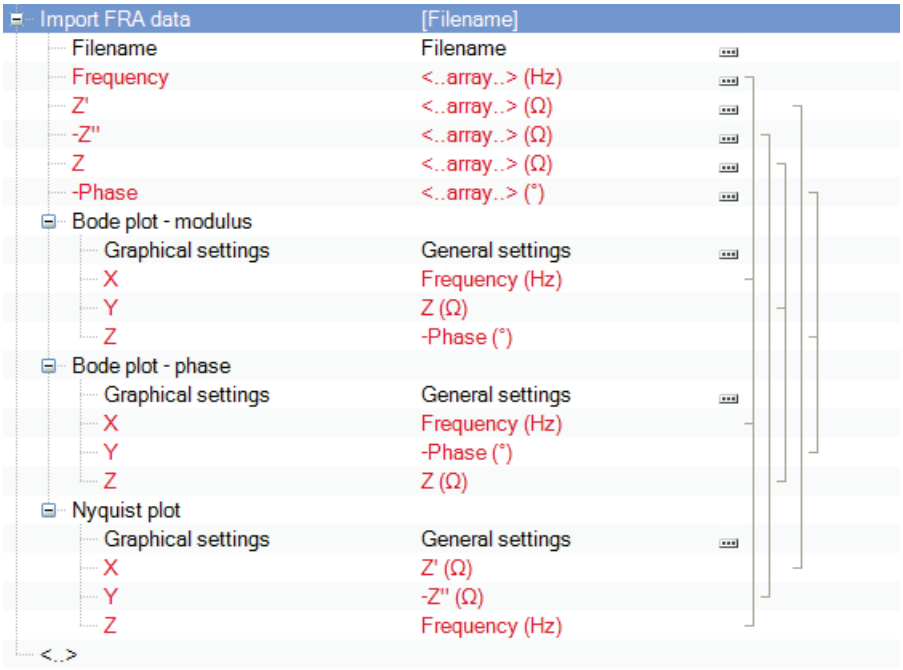


Figure 232 – The Import FRA data command

Find circle for impedance data

Analysis of the data obtained during an electrochemical impedance measurement is usually performed by fitting the experimental data with an equivalent circuit, based on the Boukamp model.

In order to help in the estimation of the parameters of the equivalent circuit, an electrochemical circle fit tool is available from the Baseline tools. This simple tool calculates the values of the elements of the equivalent circuit shown in Figure 233, using the measured data points of a circular portion of the Nyquist plot (corresponding to a single time constant).

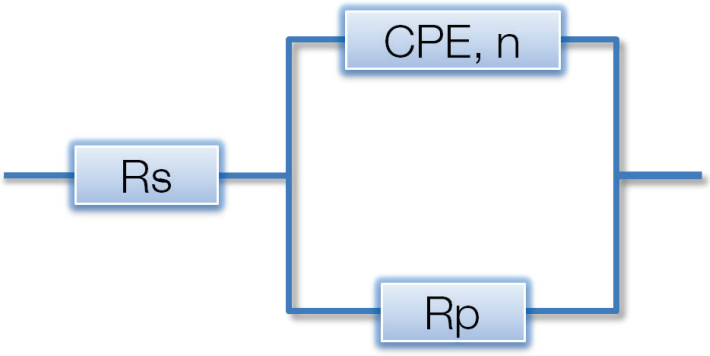


Figure 233 – The equivalent circuit used in the Electrochemical circle fit tool

This circuit includes the following items:

- Rs (Ohm) – used to simulate the value of the uncompensated resistance
- Rp (Ohm) – used to simulate the polarization resistance (also referred to as the charge transfer resistance)
- CPE – the value of the argument of the constant phase element (also referred to as a Q element)
- n – the value of the exponent of the constant phase element

To use the electrochemical circle fit, load an impedance measurement and select the Nyquist plot for display in the 2D plot area. Click on the analysis toolbar and activate the Electrochemical circle method from the Baseline fit group (see Figure 234).

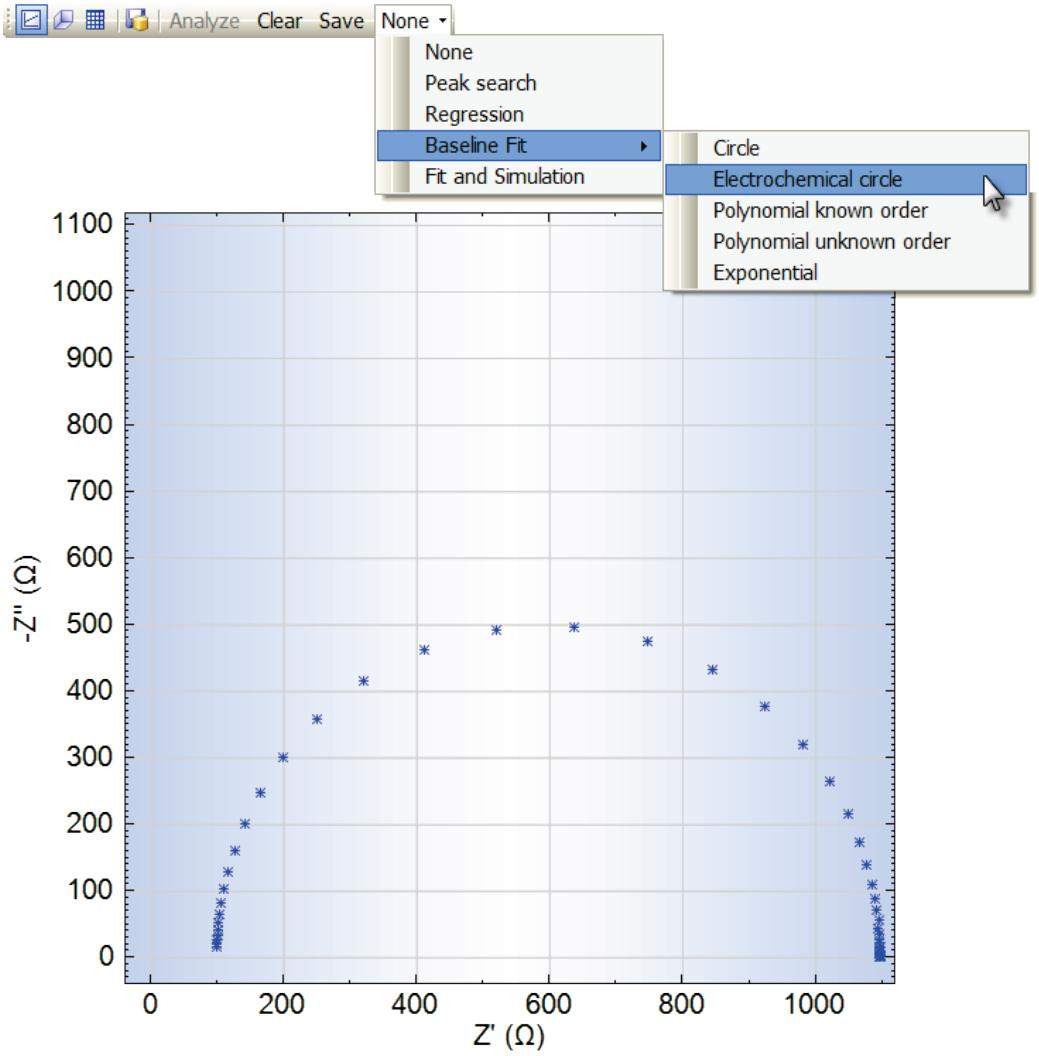


Figure 234 – Selecting the Electrochemical circle method from the Baseline fit group

Once the Electrochemical circle method has been selected, a new area will be displayed at the bottom of the 2D plot area (see Figure 235). The mouse cursor changes to a large cross.

To use the Electrochemical circle baseline fit tool, three measured data points must be clicked, fixing the data points through which the fitted circle must pass.

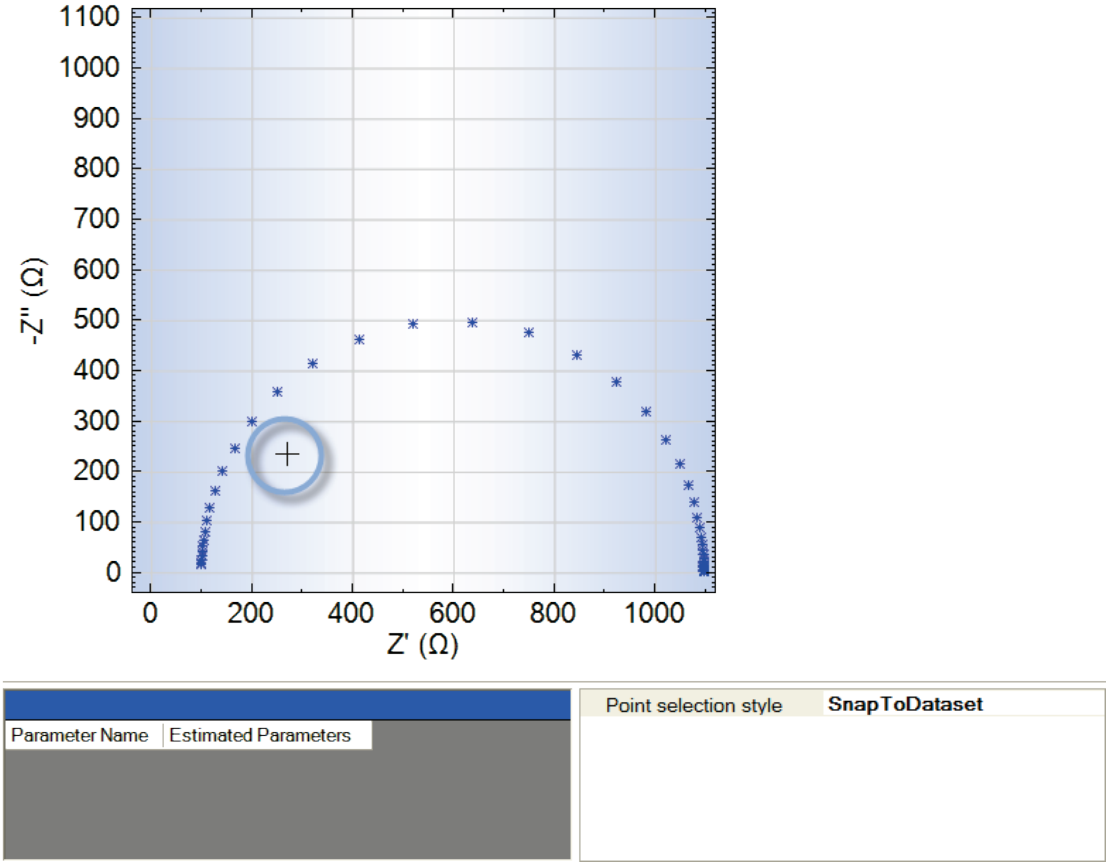


Figure 235 – Selecting the Electrochemical circle method displays a control area at the bottom of the 2D plot area

Using the left mouse button, select at least three data points in the Nyquist plot. Each selected data point will be marked by a black arrow. After the third point is clicked, the fitted circle will be plotted in the 2D plot area and the calculated values for the fitted circle will be displayed in the bottom area of the 2D plot (see Figure 236).

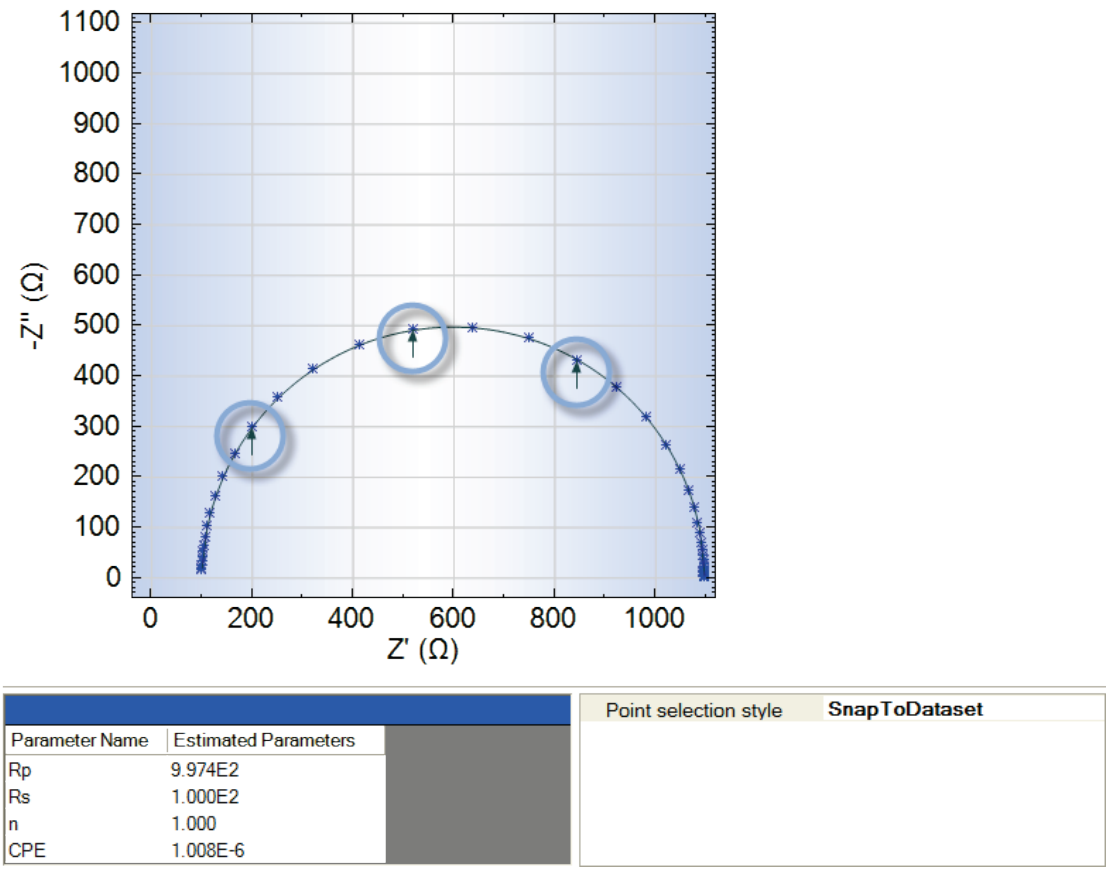


Figure 236 – The results of the Electrochemical circle fit are displayed in the area at the bottom of the 2D plot

Note: it is possible to save the results of the electrochemical circle fit by clicking the save button located in the analysis toolbar.

Fit and simulation

Detailed analysis of the data obtained during an electrochemical impedance measurement is usually performed by fitting the experimental data with an equivalent circuit, based on the Boukamp model. Many circuit elements can be used to fit the experimental data with a model. However, the equivalent circuit must be constructed carefully, since a given experimental data set can be fitted with more than one unique equivalent circuit.

The fit and simulation tool allows the definition of an equivalent circuit using the following elements:

- R, resistance
- C, capacitance
- L, inductance
- Q, constant phase element
- W, Warburg impedance
- O, Cotangent hyperbolic
- T, Tangent hyperbolic

The circuit elements can be arranged in series or in parallel. The impedance of series element is given by the sum of the impedance values of each individual element, while the impedance of the element placed in parallel is given by the reciprocal of the sum of the reciprocal impedance values of each element.

In order to use the fit and simulation tool in NOVA, load an impedance measurement and select any plot for display in the 2D plot area. Click on the analysis toolbar and activate the Fit and simulation method (see Figure 237).

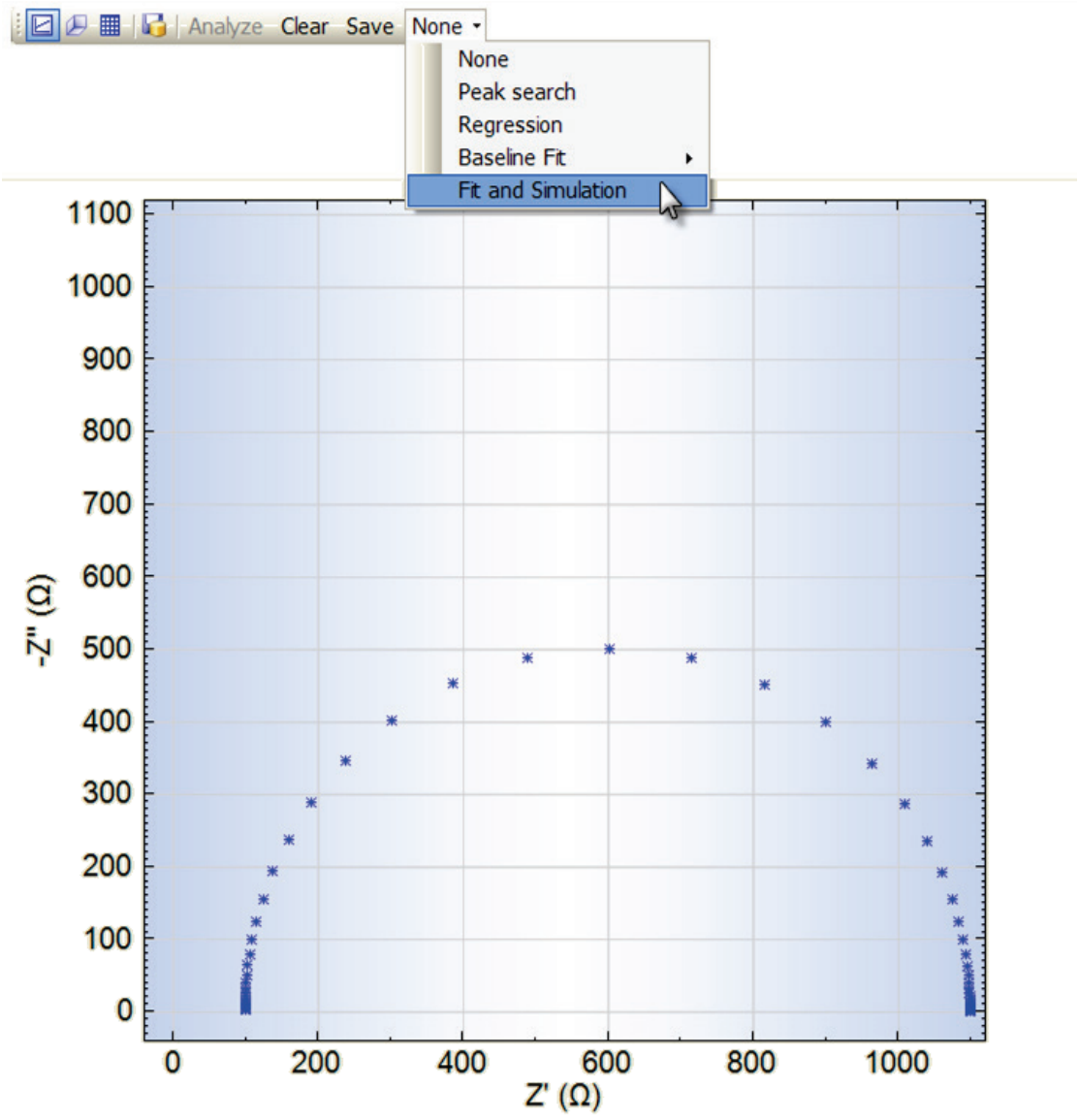


Figure 237 – Selecting the Fit and simulation tool from the Analysis toolbar

Once the Fit and simulation tool has been selected, a new area will be displayed at the bottom of the 2D plot area (see Figure 238). This area is the control interface for the fit and simulation tool.

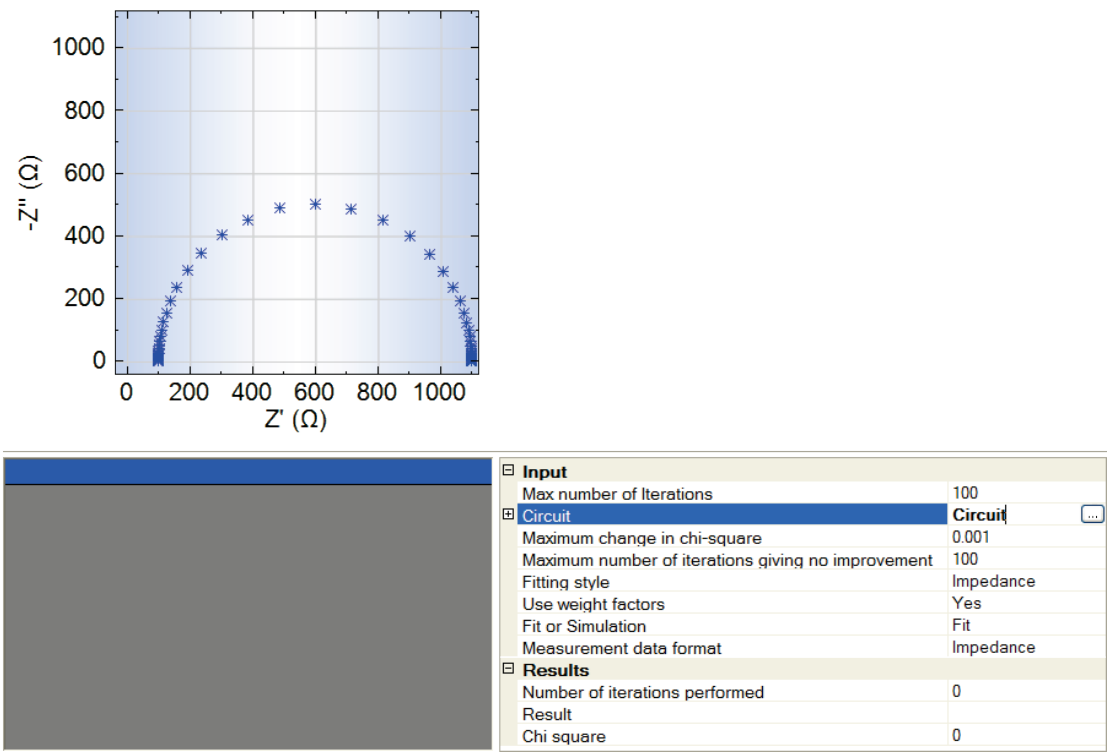


Figure 238 – Selecting the fit and simulation tool displays the large control window below the 2D plot area

The Fit and simulation control interface has a number of values and settings (see Figure 239).

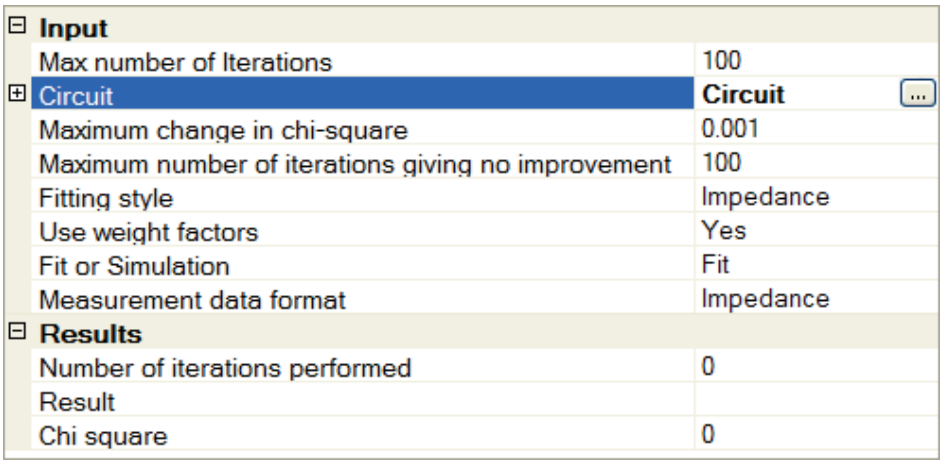


Figure 239 – The detailed view of the Fit and simulation control interface

The following parameters define the calculation method used in the fit and simulation tool:

- **Fit or Simulation:** defines the calculation method. Using the Fit methods, the software will try to find the most suitable values for the parameters of each element defined in the equivalent circuit, starting with initial, user-defined values. The simulation method simply calculates the impedance values for the equivalent circuit, as it is defined by the user.
- **Fitting style:** (impedance/admittance) – defines whether the calculation should use the impedance or the admittance values during the fit.
- **Maximum number of iterations:** defines the number of consecutive calculations used during the fitting calculation. The default value is 100.
- **Maximum change in Chi square:** defines one of the convergence criteria. The fitting will not be finished until the absolute change in the Chi square parameter (including weight factors) will be lower than this value. The default value is 0.001.
- **Maximum number of iterations giving no improvement:** defines a second stop condition for the fitting calculation. This number defines the number of iterations that are allowed during which the Chi square value does not improve. When this value is reached the fitting calculation is stopped.
- **Measurement data:** (impedance/admittance) – defines the type of data of the data set.
- **Use weight factors:** (yes / no) – defines whether a weight factor should be used during the calculation. If weight factors are used, each point is multiplied by a weight factor equal to the inverse of the square of the impedance modulus. If this option is not used, the weight factor is the same for each point, i.e. the inverse of the square root of the average of the impedance modulus.

The fit and simulation tool requires the definition of an equivalent circuit as well as initial conditions. This can be done by clicking the … button located next to the Circuit field in the fit and simulation control interface (see Figure 240).

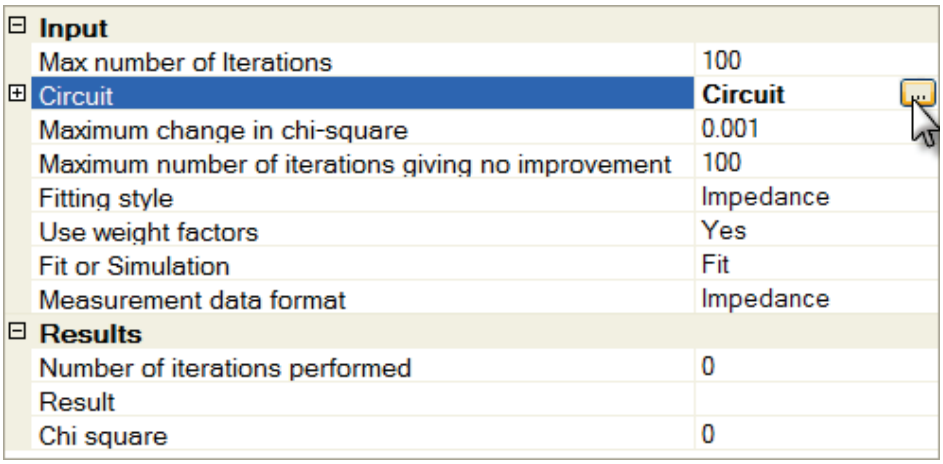


Figure 240 – Opening the circuit definition window

The circuit definition window will be displayed (see Figure 241). This window can be used to define the equivalent circuit used to fit or to simulate the data, as well as the initial conditions for the calculation.

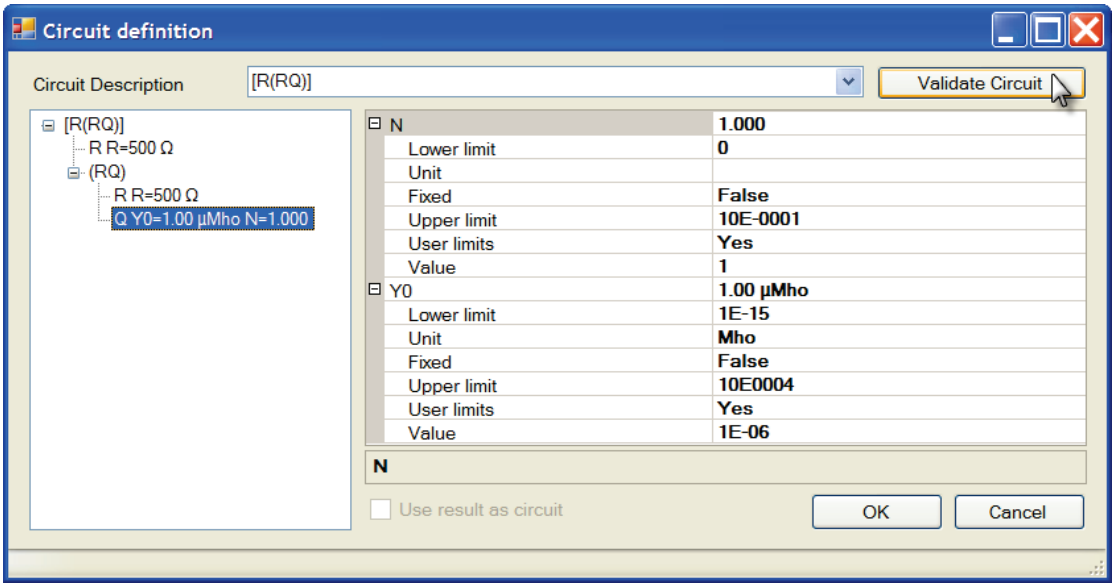


Figure 241 – The circuit definition window

To define the equivalent circuit, click the Circuit description field in the top section of the window and type the expression used to define the circuit. The following convention is used:

- Items between () are in parallel
- Items between [] are in series

For example, the equivalent circuit displayed in Figure 242, is defined by:

- R(RQ), where the first R corresponds to Rs, the second R corresponds to Rp, which is in parallel with a constant phase element, Q.

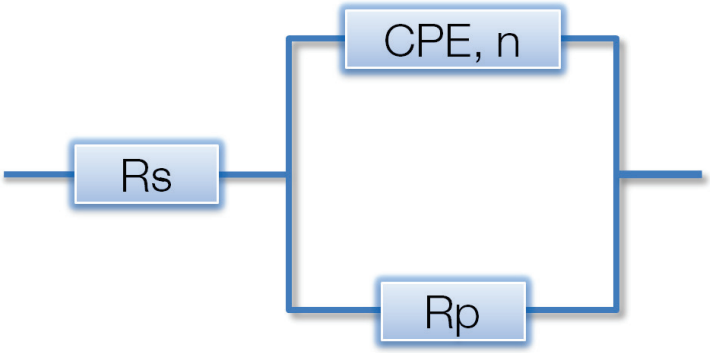


Figure 242 – A simple equivalent circuit (Randles cell)

Once the equivalent circuit is defined, click the Validate circuit button to create the circuit.

It is possible to choose an equivalent circuit from a pre-defined list of typical circuits. To do this, click the drop-down list button in the Circuit description field and select the required circuit from the list (Figure 243). Press the Validate circuit button to create the circuit.

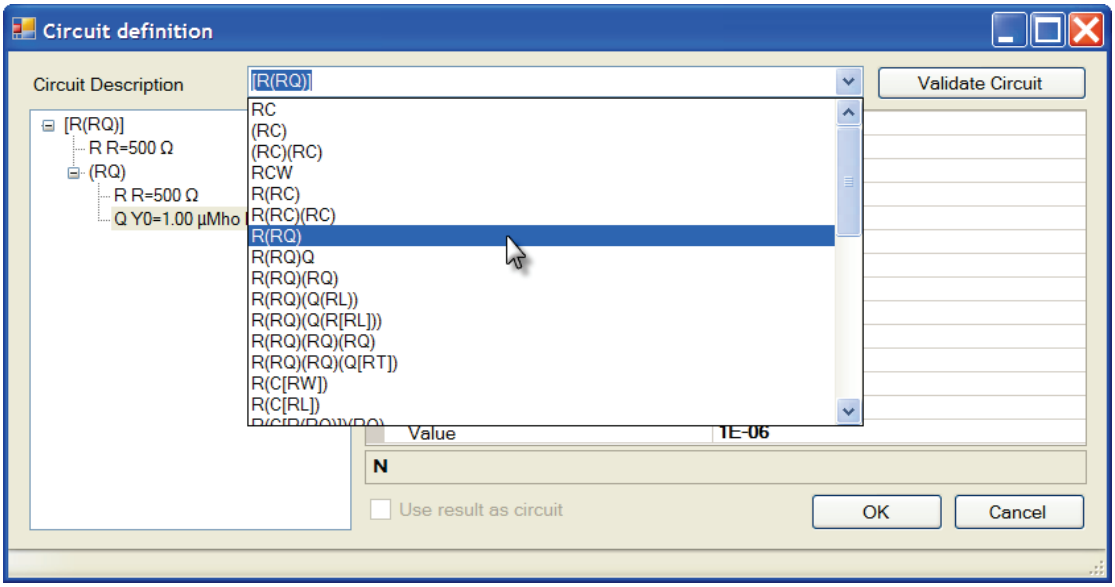


Figure 243 – Selecting an equivalent circuit from the pre-defined list

Once the equivalent circuit is defined, it is possible to define the initial values of the variable(s) of each element of the circuit. To do this, click an element in the frame on the left. The properties of the selected element will be displayed in the frame on the right (see Figure 244).

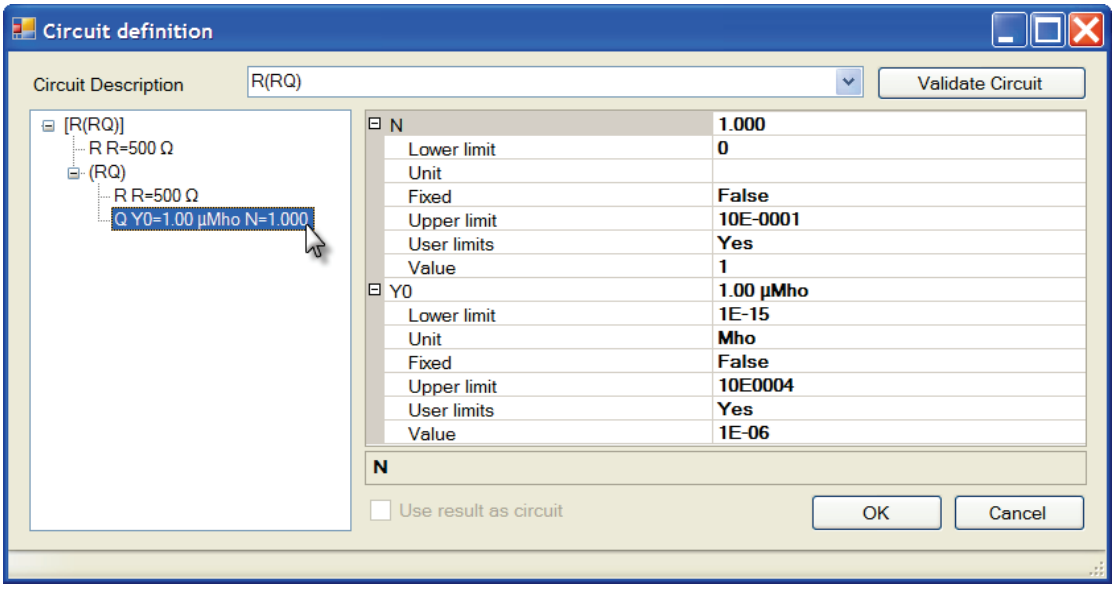


Figure 244 – Displaying the parameters and properties of the selected element (note the two variables used in the definition of the Q element)

The following settings can be edited for each individual element:

- **Lower limit:** defines the lowest possible value for the variable of the element, to be used during the fitting of the data.
- **Unit:** defines the unit used for the element.
- **Fixed:** (true/false) – defines whether the value of the variable can be changed during the fitting of the data. The default setting is false.
- **Upper limit:** defines the highest possible value for the variable of the element, to be used during the fitting of the data.
- **User limits:** (yes/no) – defines whether the Lower and Upper limit should be used during the fitting of the data. Default setting is yes.
- **Value:** defines the initial value of the variable of the circuit element.

Note: some circuit elements have more than one variable. The fitting parameters can be defined for each variable, independently (see Figure 244).

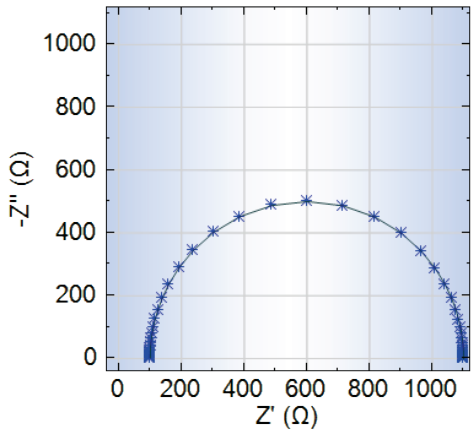
Once the fitting conditions have been defined, the calculation can be performed.

Fitting the data using an equivalent circuit

To start the fitting algorithm, click the Analyze button located in the toolbar. This will start the calculation, using the defined equivalent circuit and the initial conditions for each element.

If the fitting calculation succeeds, the calculated data points will be plotted in the 2D plot area, overlaying the original data set (see Figure 245). The area below the 2D plot area is updated after the calculation. A table is displayed on the left hand side, showing the calculated values of the total impedance, the real and imaginary components and the phase angle (see Figure 245). The Fit and simulation control

interface is also updated and displays the number of iterations required to reach the final result and the final value of the Chi square parameter (χ^2).



Modulus	Imaginary	Phase	Real
100.01515328	-1.591569073	-0.91180223	100.002488939
100.02404264	-2.003654954	-1.14781055	100.003972291
100.03813061	-2.522489929	-1.44488252	100.006322905
100.06045162	-3.175597688	-1.81868959	100.010047285
100.09581406	-3.997751186	-2.28895895	100.015948625
100.15183718	-5.032854396	-2.88045459	100.025301143
100.24056030	-6.335921665	-3.62391955	100.040122086
100.38099991	-7.976190686	-4.55747935	100.063607403
100.60316599	-10.04100996	-5.72811962	100.100824806
100.95426806	-12.64030497	-7.19278081	100.159806960

Input	
Max number of Iterations	100
Circuit	**Circuit**
Maximum change in chi-square	0.001
Maximum number of iterations giving no improvement	100
Fitting style	Impedance
Use weight factors	Yes
Fit or Simulation	**Fit**
Measurement data format	Impedance
Results	
Number of iterations performed	**5**
Result	**Circuit**
Chi square	**3.8E-10**

Figure 245 – The 2D plot area is updated after the fit (the black line plot corresponds to the calculated data)

To view the fitted circuit elements, click the … button located next to the Result field in the fit and simulation control interface (see Figure 246).

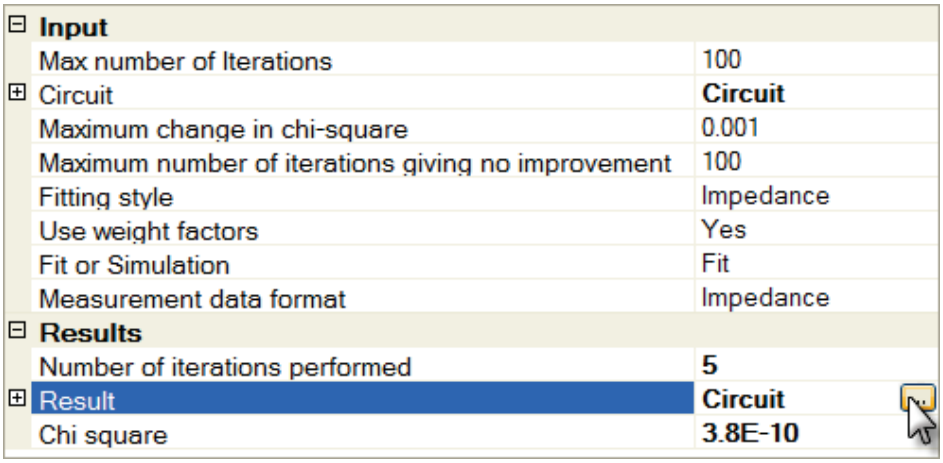


Figure 246 – Opening the results window

This opens a new window, similar to the one used to create the equivalent circuit (see Figure 247). The calculated values and the estimated error are displayed for each element.

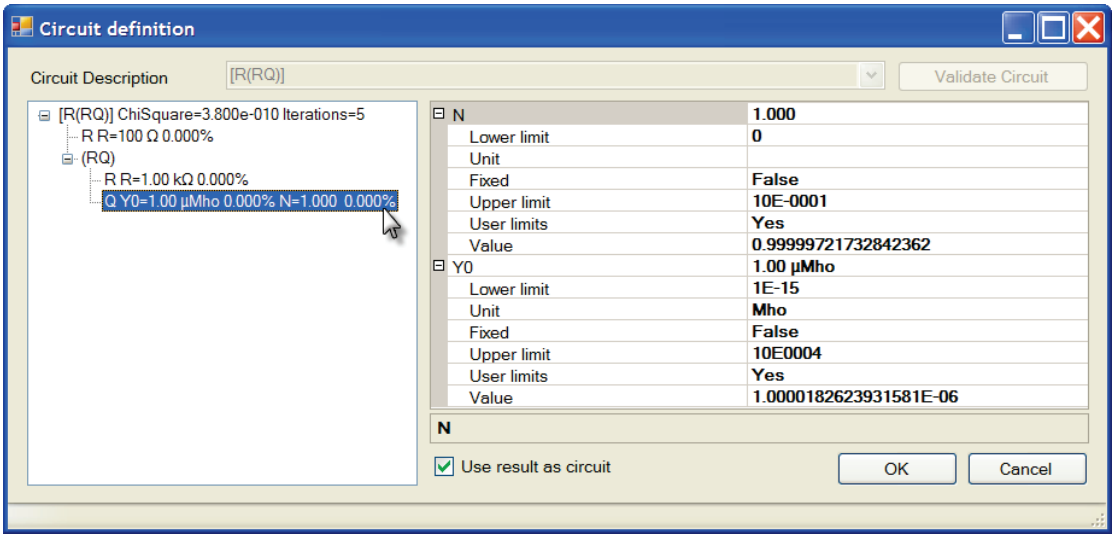


Figure 247 – The detailed results of the fit calculation

The frame on the right displays the detailed calculated values of each variable for the selected element.

Note: if the fit calculation is not complete after the maximum number of iterations, it is possible to resume the fitting using the last calculated values of each element of the equivalent circuit. To do this, check the 'Use result as circuit' check box in the Results window and press the analyze button to restart the fit calculation, using the last values as initial conditions (see Figure 247).

To save the results of the fitting, click the Save button located in the toolbar. This will add the calculation to the data set, which will be available as a new signal set in the data explorer (see Figure 248).

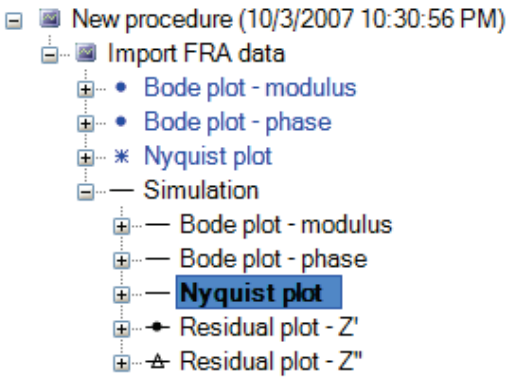


Figure 248 – The saved results of the fit are added to the data set

The added signal set contains the calculated Bode and Nyquist plots, as well as the residual plots for Z' and Z".

Simulating the data using an equivalent circuit

The simulation tool can be used to calculate the expected behavior of a user-defined equivalent circuit. To use the simulation tool, the equivalent circuit must first be defined, in the same way as for the fitting procedure. However, the Fit or Simulation parameter in the control interface must be set to Simulation (see Figure 249).

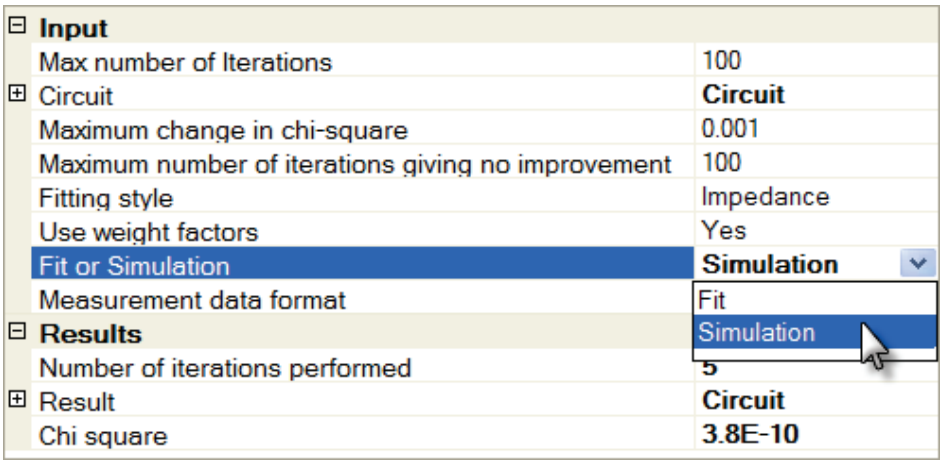
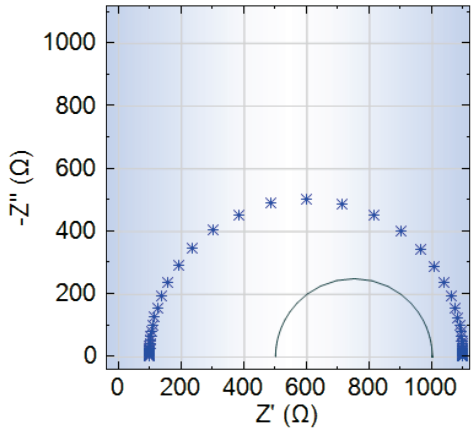


Figure 249 – To use the simulation tool, the Fit or Simulation parameter must be set accordingly

To start the simulation algorithm, click the Analyze button located in the toolbar. This will calculate the expected behavior of the equivalent circuit, using the initial parameters for each of the circuit elements. Figure 250 shows an example of simulated data.



Modulus	Imaginary	Phase	Real
500.00759889	-1.59152693	-0.182373089	500.00506596
500.01204321	-2.00359429	-0.229590078	500.00802890
500.01908758	-2.52239742	-0.289035645	500.01272530
500.03025071	-3.17544783	-0.363859949	500.02016775
500.04794065	-3.99749440	-0.458040077	500.03196196
500.07597687	-5.03239327	-0.576591909	500.05065509
500.12040393	-6.33506375	-0.725789471	500.08027895
500.19079270	-7.97455430	-0.913506746	500.12721940
500.30230501	-10.0378363	-1.149633422	500.20159760
500.47893697	-12.6340838	-1.446527582	500.31944423

Input	
Max number of Iterations	100
Circuit	**Circuit**
Maximum change in chi-square	0.001
Maximum number of iterations giving no improvement	100
Fitting style	Impedance
Use weight factors	Yes
Fit or Simulation	**Simulation**
Measurement data format	Impedance
Results	
Number of iterations performed	**5**
Result	**Circuit**
Chi square	**3.8E-10**

Figure 250 – The results of the simulation are displayed in the same way as those of the fitting

The results of the simulation are displayed in the same way as those of the fitting calculation. Clicking the Save button, located in the toolbar, will save the results of the simulation.